

# Assessment of the Potential Impacts of Hydraulic Fracturing for Oil and Gas on Drinking Water Resources

## *Appendices A-J*

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# **Assessment of the Potential Impacts of Hydraulic Fracturing for Oil and Gas on Drinking Water Resources (Appendices A – J)**

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Office of Research and Development  
U.S. Environmental Protection Agency  
Washington, DC 20460

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**Contents: Appendices****Appendix A. Chemicals Identified in Hydraulic Fracturing Fluids and/or Flowback and****Produced Water**

A.1. Supplemental Tables and Information .....	A-1
Table A-1. Description of sources used to create lists of chemicals used in fracturing fluids or detected in flowback or produced water. ....	A-1
Table A-2. Chemicals reported to be used in hydraulic fracturing fluids. ....	A-4
Table A-3. List of generic names of chemicals reportedly used in hydraulic fracturing fluids. ....	A-46
Table A-4. Chemicals detected in flowback or produced water. ....	A-58
A.2. References for Appendix A .....	A-63

**Appendix B. Water Acquisition Tables .....** B-1

B.1. Supplemental Tables .....	B-1
Table B-1. Annual average hydraulic fracturing water use and consumption in 2011 and 2012 compared to total annual water use and consumption in 2010 by state. ....	B-1
Table B-2. Annual average hydraulic fracturing water use and consumption in 2011 and 2012 compared to total annual water use and consumption in 2010 by county. ....	B-3
Table B-3. Comparison of water use per well estimates from the EPA’s project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) and literature sources. ....	B-20
Table B-4. Comparison of well counts from the EPA’s project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) and state databases for North Dakota, Pennsylvania, and West Virginia. ....	B-21
Table B-5. Water use per hydraulically fractured well as reported in the EPA’s project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) by state and basin. ....	B-22
Table B-6. Estimated percent domestic use water from ground water and self-supplied by county. ....	B-26
Table B-7. Projected hydraulic fracturing water use by Texas counties between 2015 and 2060, expressed as a percentage of 2010 total county water use. ....	B-40
B.2. References for Appendix B .....	B-52

**Appendix C. Chemical Mixing Supplemental Tables and Information .....** C-1

C.1. Supplemental Tables and Information .....	C-1
Table C-1. Chemicals reported to FracFocus in 10% or more of disclosures for gas-producing wells, with the number of disclosures where chemical is reported, percentage of disclosures, and the median maximum concentration (% by mass) of that chemical in hydraulic fracturing fluid. ....	C-1
Table C-2. Chemicals reported to FracFocus in 10% or more of disclosures for oil-producing wells, with the number of disclosures where chemical is reported, percentage of disclosures, and the median maximum concentration (% by mass) of that chemical in hydraulic fracturing fluid. ....	C-3
Table C-3a. Top chemicals reported to FracFocus for each state and number (and percentage) of disclosures where a chemical is reported for that state, Alabama to Montana (U.S. EPA, 2015c). ....	C-5

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Table C-3b. Top chemicals reported to FracFocus for each state and number (and percentage) of disclosures where a chemical is reported for that state, New Mexico to Wyoming (U.S. EPA, 2015c). ..... C-12

Table C-4. Estimated mean, median, 5<sup>th</sup> percentile, and 95<sup>th</sup> percentile volumes in gallons for chemicals reported to FracFocus in 100 or more disclosures, where density information was available. .... C-20

Table C-5. Estimated mean, median, 5<sup>th</sup> percentile, and 95<sup>th</sup> percentile volumes in liters for chemicals reported to FracFocus in 100 or more disclosures, where density information was available. .... C-23

Table C-6. Calculated mean, median, 5<sup>th</sup> percentile, and 95<sup>th</sup> percentile chemical masses reported to FracFocus in 100 or more disclosures, where density information was available... C-26

Table C-7. Associated chemical densities and references used to calculate chemical mass and estimate chemical volume..... C-29

Table C-8. Selected physicochemical properties of chemicals reported as used in hydraulic fracturing fluids. .... C-32

C.2. References for Appendix C ..... C-76

**Appendix D. Designing, Constructing, and Testing Wells for Integrity ..... D-1**

D.1. Design Goals for Well Construction..... D-1

D.2. Well Components ..... D-1

Text Box D-1. Selected Industry-Developed Specifications and Recommended Practices for Well Construction in North America..... D-2

D.2.1. Casing ..... D-2

D.2.2. Cement ..... D-3

Figure D-1. A typical staged cementing process. .... D-8

D.3. Well Completions ..... D-9

Figure D-2. Examples of well completion types. .... D-9

D.4. Mechanical Integrity Testing ..... D-10

D.4.1. Internal Mechanical Integrity ..... D-11

D.4.2. External Mechanical Integrity ..... D-12

D.5. References for Appendix D..... D-13

**Appendix E. Flowback and Produced Water Supplemental Tables and Information ..... E-1**

E.1. Flowback and Long-Term Produced Water Volumes .....E-1

Table E-1. Flowback and long-term produced water characteristics for wells in unconventional formations, formation-level data. ....E-2

E.2. Produced Water Content .....E-6

E.2.1. Introduction.....E-6

E.2.2. General Water Quality Parameters .....E-6

Table E-2. Reported concentrations of general water quality parameters in produced water for unconventional shale and tight formations, presented as: average (minimum–maximum) or *median* (minimum–maximum).....E-7

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Table E-3. Reported concentrations of general water quality parameters in produced water for unconventional coalbed basins, presented as: average (minimum–maximum). ..... E-10

E.2.3. Salinity and Inorganics..... E-11

Table E-4. Reported concentrations (mg/L) of inorganic constituents contributing to salinity in unconventional shale and tight formations produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum)..... E-12

Table E-5. Reported concentrations (mg/L) of inorganic constituents contributing to salinity in produced water for unconventional CBM basins, presented as: average (minimum–maximum). ..... E-14

E.2.4. Metals and Metalloids..... E-14

Table E-6. Reported concentrations (mg/L) of metals and metalloids from unconventional shale and tight formation produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum). ..... E-15

Table E-7. Reported concentrations (mg/L) of metals and metalloids from unconventional coalbed produced water, presented as: average (minimum–maximum). ..... E-18

E.2.5. Naturally Occurring Radioactive Material (NORM) and Technically Enhanced Naturally Occurring Radioactive Material (TENORM) ..... E-20

Table E-8. Reported concentrations (in pCi/L) of radioactive constituents in unconventional shale and sandstone produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum). ..... E-22

E.2.6. Organics..... E-24

Table E-9. Concentrations of select organic parameters from unconventional shale, a tight formation, and coalbed produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum). ..... E-25

Table E-10. Reported concentrations (µg/L) of organic constituents in produced water for two unconventional shale formations, presented as: average (minimum–maximum) or *median* (minimum–maximum). ..... E-28

Table E-11. Reported concentrations of organic constituents in 65 samples of produced water from the Black Warrior CBM Basin, presented as average (minimum–maximum)..... E-30

E.2.7. Chemical Reactions ..... E-31

E.2.8. Microbial Community Processes and Content ..... E-32

E.3. Produced Water Content Spatial Trends ..... E-34

E.3.1. Variability between Plays of the Same Rock Type..... E-34

E.3.2. Local Variability ..... E-36

E.4. Example Calculation for Roadway Transport ..... E-36

E.4.1. Estimation of Transport Distance ..... E-36

E.4.2. Estimation of Wastewater Volumes..... E-37

E.4.3. Estimation of Roadway Accidents ..... E-37

Table E-12. Combination truck crashes in 2012 for the 2,469,094 registered combination trucks, which traveled 163,458 million miles (U.S. Department of Transportation, 2012).<sup>a</sup> ... E-37

Table E-13. Large truck crashes in 2012 (U.S. Department of Transportation, 2012).<sup>a</sup> ..... E-38

E.4.4. Estimation of Material Release Rates in Crashes ..... E-38

E.4.5. Estimation of Volume Released in Accidents ..... E-38

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Table E-14. Estimate of total truck-travel miles per well in the Susquehanna River Basin based on the transport analysis performed by Gilmore et al. (2013). ..... E-39

E.5. References for Appendix E ..... E-39

**Appendix F. Wastewater Treatment and Waste Disposal Supplemental Information ..... F-1**

F.1. Estimates of Wastewater Production in Regions where Hydraulic Fracturing is Occurring.....F-1

    Table F-1. Estimated volumes (millions of gallons) of wastewater based on state data for selected years and numbers of wells producing fluid.....F-2

F.2. Overview of Treatment Processes for Treating Hydraulic Fracturing Wastewater.....F-6

    F.2.1. Basic Treatment.....F-6

        Figure F-1. Electrocoagulation unit. ....F-7

    F.2.2. Advanced Treatment.....F-8

        Figure F-2. Photograph of reverse osmosis system. ....F-9

        Figure F-3. Picture of mobile electro dialysis units in Wyoming. ....F-10

        Figure F-4. Picture of a mechanical vapor recompression unit near Decatur, Texas. ....F-11

        Figure F-5. Mechanical vapor recompression process design – Maggie Spain Facility. ....F-12

        Figure F-6. Picture of a compressed bed ion exchange unit. ....F-13

        Figure F-7. Discharge water process used in the Pinedale Anticline field.....F-14

F.3. Treatment Technology Removal Capabilities .....F-14

    Table F-2. Removal efficiency of different hydraulic fracturing wastewater constituents using various wastewater treatment technologies.<sup>a</sup> .....F-15

    Table F-3. Treatment processes for hydraulic fracturing wastewater organic constituents. ....F-18

    Table F-4. Estimated effluent concentrations for example constituents based on treatment process removal efficiencies.....F-20

F.4. Centralized Waste Treatment Facilities and Waste Management Options .....F-23

    F.4.1. Discharge Options for CWTs.....F-23

F.5. Water Quality for Reuse .....F-24

    Table F-5. Water quality requirements for reuse.....F-24

    Figure F-8. Diagram of treatment for reuse of flowback and produced water.....F-26

F.6. Hydraulic Fracturing Impacts on POTWs .....F-27

    F.6.1. Potential Impacts on Treatment Processes.....F-27

F.7. Hydraulic Fracturing and DBPs .....F-27

F.8. References for Appendix F .....F-28

**Appendix G. Identification and Hazard Evaluation of Chemicals across the Hydraulic Fracturing Water Cycle Supplemental Tables and Information .....G-1**

G.1. Criteria for Selection and Inclusion of Reference Value (RfV) and Oral Slope Factor (OSF) Data Sources G-1

    G.1.1. Included Sources .....G-3

    G.1.2. Excluded Sources.....G-3

G.2. Glossary of Toxicity Value Terminology.....G-4

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G.3. Tables ..... G-9

    Table G-1a. Chemicals reported to be used in hydraulic fracturing fluids, with available federal chronic RfVs and OSFs. .... G-9

    Table G-1b. Chemicals reported to be used in hydraulic fracturing fluids, with available state chronic RfVs and OSFs. .... G-18

    Table G-1c. Chemicals reported to be used in hydraulic fracturing fluids, with available international chronic RfVs and OSFs. .... G-19

    Table G-1d. Chemicals reported to be used in hydraulic fracturing fluids, with available less-than-chronic RfVs and OSFs. .... G-20

    Table G-2a. Chemicals reported to be detected in flowback or produced water, with available federal chronic RfVs and OSFs. .... G-23

    Table G-2b. Chemicals reported to be detected in flowback or produced water, with available state chronic RfVs and OSFs. .... G-31

    Table G-2c. Chemicals reported to be detected in flowback or produced water, with available international chronic RfVs and OSFs. .... G-33

    Table G-2d. Chemicals reported to be detected in flowback or produced water, with available less-than-chronic RfVs and OSFs. .... G-34

G.4. References for Appendix G ..... G-36

**Appendix H. Description of EPA Hydraulic Fracturing Study Publications Cited in This Assessment ..... H-1**

    Table H-1. Titles, descriptions, and citations for EPA hydraulic fracturing study publications cited in this assessment. .... H-1

**Appendix I. Unit Conversions ..... I-1**

**Appendix J. Glossary ..... J-1**

    J.1. Glossary Terms and Definitions ..... J-1

    J.2. References for Appendix J ..... J-17

## Appendix A

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# Chemicals Identified in Hydraulic Fracturing Fluids and/or Flowback and Produced Water

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# Appendix A. Chemicals Identified in Hydraulic Fracturing Fluids and/or Flowback and Produced Water

## A.1. Supplemental Tables and Information

1 The EPA identified authoritative sources for information on hydraulic fracturing chemicals and, to  
 2 the extent possible, verified the chemicals used in hydraulic fracturing fluids and detected in  
 3 flowback and produced water of hydraulically fractured wells. The EPA used 10 sources to identify  
 4 the chemicals used in hydraulic fracturing fluids or detected in flowback or produced water. Seven  
 5 sources are government entities (Congressional, federal, or state) that obtained the data directly  
 6 from industry. The remaining three represent collaborations between state, non-profit, academic,  
 7 and industry groups. FracFocus is the result of a collaboration between the Ground Water  
 8 Protection Council (a non-profit coalition of state ground water protection agencies) and  
 9 the Interstate Oil and Gas Compact Commission (a multi-state government agency). The Marcellus  
 10 Shale Coalition is a drilling industry trade group. [Colborn et al. \(2011\)](#) is a peer-reviewed journal  
 11 article. Most of the listed chemicals were cited by multiple sources.

12 Seven of the ten sources obtained information about the chemicals used in hydraulic fracturing  
 13 fluids from material safety data sheets (MSDSs) provided by chemical manufacturers for the  
 14 products they sell, as required by the Occupational Safety and Health Administration (OSHA). The  
 15 MSDSs must list all hazardous ingredients if they comprise at least 1% of the product; for  
 16 carcinogens, the reporting threshold is 0.1%. However, chemical manufacturers may withhold  
 17 information (e.g., chemical name, concentration of the substance in a mixture) about a hazardous  
 18 substance from MSDSs if it is claimed as confidential business information (CBI), provided that  
 19 certain conditions are met ([OSHA, 2013](#)).

**Table A-1. Description of sources used to create lists of chemicals used in fracturing fluids or detected in flowback or produced water.**

The number next to each citation in the reference column corresponds to numbers in the reference columns found in Table A-2, Table A-3, and Table A-4.

Description / Content	Reference
Chemicals and other components used by 14 hydraulic fracturing service companies from 2005 to 2009 as reported to the House Committee on Energy and Commerce. For each hydraulic fracturing product reported, companies also provided an MSDS with information about the product's chemical components.	<a href="#">House of Representatives (2011)<sup>a</sup> (1)</a>

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Description / Content	Reference
Chemicals used during natural gas operations with some potential health effects. The list of chemicals was compiled from MSDSs from several sources, including the Bureau of Land Management, U.S. Forest Service, state agencies, and industry.	<a href="#">Colborn et al. (2011)<sup>a</sup></a> (2)
Chemicals used or proposed for use in hydraulic fracturing in the Marcellus Shale in New York based on product composition disclosures and MSDSs submitted to the New York State Department of Environmental Conservation (NYSDEC). Also includes data provided separately to NYSDEC by well operators on analytical results of flowback water samples from Marcellus Shale operations in Pennsylvania and West Virginia.	<a href="#">NYSDEC (2011)<sup>a,b</sup></a> (3)
Chemicals reported to be used by nine hydraulic fracturing service companies from 2005 to 2010. Companies provided the chemical names in MSDSs, product bulletins, and formulation sheets.	<a href="#">U.S. EPA (2013a)<sup>a</sup></a> (4)
MSDSs provided to the EPA during on-site visits to hydraulically fractured oil and gas wells in Oklahoma and Colorado.	<a href="#">Sheets</a>
Characteristics of undiluted chemicals found in hydraulic fracturing fluids associated with coalbed methane production, based on MSDSs, literature searches, reviews of relevant MSDSs provided by service companies, and discussions with field engineers, service company chemists, and state and federal employees.	<a href="#">U.S. EPA (2004)<sup>a</sup></a> (6)
Chemicals used in Pennsylvania for hydraulic fracturing activities based on MSDSs provided by industry.	<a href="#">PA DEP (2010)<sup>a</sup></a> (7)
Chemical records entered in FracFocus by oil and gas operators for individual wells from January 1, 2011, through February 28, 2013. FracFocus is a publicly accessible hydraulic fracturing chemical registry developed by the Ground Water Protection Council and the Interstate Oil and Gas Compact Commission. Chemicals claimed as confidential business information (CBI) do not have to be reported in FracFocus.	<a href="#">U.S. EPA (2015c)<sup>a</sup></a> (8)
Chemicals detected in flowback from 19 hydraulically fractured shale gas wells in Pennsylvania and West Virginia, based on analyses conducted by 17 Marcellus Shale Coalition member companies.	<a href="#">Hayes (2009)<sup>b</sup></a> (9)
Chemicals reportedly detected in flowback and produced water from 81 wells provided to the EPA by nine well operating companies.	<a href="#">U.S. EPA (2011b)<sup>b</sup></a> (10)

<sup>a</sup> Sources used to identify chemicals used in hydraulic fracturing fluids.

<sup>b</sup> Sources used to identify chemicals detected in flowback and produced water.

- 1 Once it had identified chemicals used in hydraulic fracturing fluids and chemicals detected in
- 2 flowback/produced water, the EPA conducted an initial review of the chemicals for preliminary
- 3 validation of provided chemical name and Chemical Abstracts Service Registry Number (CASRN)
- 4 combinations. A CASRN is a unique numeric identifier assigned by the Chemical Abstracts Service
- 5 (CAS) to a chemical substance when it enters the CAS Registry Database. The EPA Office of Research

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1 and Development's National Center for Computational Toxicology (NCCT) provided the final formal  
2 validation and verification of the listed chemicals.

3 The EPA first compared the hydraulic fracturing chemical CASRN and names with chemicals listed  
4 in NCCT's Distributed Structure-Searchable Toxicity Database network (DSSTox) database ([U.S.  
5 EPA, 2013b](#)). For the CASRN and chemical names that did not appear in the DSSTox database, the  
6 EPA's Substance Registry Services database and the U.S. National Library of Medicine ChemID  
7 database were used to verify accurate chemical name and CASRN pairing ([NLM, 2014](#); [U.S. EPA,  
8 2014c](#)). The EPA also identified cases where CASRN/name combinations could not be verified by  
9 use of selected public sources and flagged those cases for resolution by NCCT.

10 NCCT then verified all of the CASRN and chemical names for the chemical lists generated by the EPA  
11 in accordance with NCCT DSSTox Chemical Information Quality Review Procedures  
12 (<http://www.epa.gov/ncct/dsstox/ChemicalInfQAProcedures.html>). The process included QA/QC  
13 on the identification and validation of CASRN/chemical name combinations and resolution of  
14 inconsistencies and problems including duplications, CASRN errors, and CASRN/chemical name  
15 mismatches.

16 The general methodology for resolving conflicts between CASRN/chemical name combinations and  
17 other chemical identification issues differed slightly depending on the data provided by each  
18 source. To resolve chemical/CASRN conflict in data provided by the nine service companies, the  
19 EPA worked with each company to verify the CASRN/chemical combinations proposed by NCCT. In  
20 cases of CASRN/chemical name mismatches in data provided by FracFocus, chemical names were  
21 considered primary to the CASRN (i.e., the name overrode the CASRN). When the chemical name  
22 was non-specific and the CASRN was valid, then the CASRN was considered primary to the chemical  
23 name, and the correct specific chemical name from DSSTox was assigned to the CASRN. For all other  
24 sources, the CASRN was considered primary unless it was invalid or missing. In such cases, the  
25 chemical name was primary. All Toxic Substance Control Act (TSCA) CBI chemical lists were  
26 managed in accordance with TSCA CBI procedures.

27 Chemicals with verified CASRN that are used in hydraulic fracturing fluids are presented in Table  
28 A-2. Generic chemicals used in hydraulic fracturing fluids are presented in Table A-3. Chemicals  
29 with verified CASRN that have been detected in flowback or produced water are presented in  
30 Table A-4. Chemicals found in both fracturing fluids (see Table A-2) and flowback and produced  
31 water (see Table A-4) are italicized in each table.

**Table A-2. Chemicals reported to be used in hydraulic fracturing fluids.**

An “X” indicates the availability of physicochemical properties from EPI Suite™ (see Appendix C) and selected toxicity reference values (see Appendix G). An empty cell indicates no information was available from the sources we consulted. Reference number corresponds to the citations in Table A-1. Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
(13Z)-N,N-bis(2-hydroxyethyl)-N-methyldocos-13-en-1-aminium chloride	120086-58-0	X		1
(2,3-dihydroxypropyl)trimethylammonium chloride	34004-36-9	X		8
(E)-Crotonaldehyde	123-73-9	X	X	1, 4
[Nitrilotris(methylene)]tris-phosphonic acid pentasodium salt	2235-43-0	X		1
1-(1-Naphthylmethyl)quinolinium chloride	65322-65-8	X		1
1-(Alkyl* amino)-3-aminopropane *(42%C12, 26%C18, 15%C14, 8%C16, 5%C10, 4%C8)	68155-37-3	X		8
1-(Phenylmethyl)pyridinium Et Me derivs., chlorides	68909-18-2	X		1, 2, 3, 4, 6, 8
1,2,3-Trimethylbenzene	526-73-8	X		1, 4
<i>1,2,4-Trimethylbenzene</i>	<i>95-63-6</i>	X		<i>1, 2, 3, 4, 5</i>
1,2-Benzisothiazolin-3-one	2634-33-5	X		1, 3, 4
1,2-Dibromo-2,4-dicyanobutane	35691-65-7	X		1, 4
1,2-Dimethylbenzene	95-47-6	X		4
1,2-Ethanediamine, polymer with 2-methyloxirane	25214-63-5			8
1,2-Ethanediaminium, N,N'-bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'-bis(2-hydroxyethyl)-N,N'-dimethyl-, tetrachloride	138879-94-4	X		1, 4
<i>1,2-Propylene glycol</i>	<i>57-55-6</i>	X	X	<i>1, 2, 3, 4, 8</i>
1,2-Propylene oxide	75-56-9	X	X	1, 4
1,3,5-Triazine	290-87-9	X		8
1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol	4719-04-4	X		1, 4
<i>1,3,5-Trimethylbenzene</i>	<i>108-67-8</i>	X		<i>1, 4</i>
1,3-Butadiene	106-99-0	X	X	8

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
1,3-Dichloropropene	542-75-6	X	X	8
1,4-Dioxane	123-91-1	X	X	2, 3, 4
1,4-Dioxane-2,5-dione, 3,6-dimethyl-, (3R,6R)-, polymer with (3S,6S)-3,6-dimethyl-1,4-dioxane-2,5-dione and (3R,6S)-rel-3,6-dimethyl-1,4-dioxane-2,5-dione	9051-89-2			1, 4, 8
1,6-Hexanediamine	124-09-4	X		1, 2
1,6-Hexanediamine dihydrochloride	6055-52-3	X		1
1-[2-(2-Methoxy-1-methylethoxy)-1-methylethoxy]-2-propanol	20324-33-8	X		4
1-Amino-2-propanol	78-96-6	X		8
1-Benzylquinolinium chloride	15619-48-4	X		1, 3, 4
1-Butanol	71-36-3	X	X	1, 2, 3, 4, 7
1-Butoxy-2-propanol	5131-66-8	X		8
1-Decanol	112-30-1	X		1, 4
1-Dodecyl-2-pyrrolidinone	2687-96-9	X		1, 4
1-Eicosene	3452-07-1	X		3
1-Ethyl-2-methylbenzene	611-14-3	X		4
1-Hexadecene	629-73-2	X		3
1-Hexanol	111-27-3	X		1, 4, 8
1-Hexanol, 2-ethyl-, manuf. of, by products from, distn. residues	68909-68-7			4
1H-Imidazole-1-ethanamine, 4,5-dihydro-, 2-nortall-oil alkyl derivs.	68442-97-7			2, 4
1-Methoxy-2-propanol	107-98-2	X		1, 2, 3, 4
1-Octadecanamine, acetate (1:1)	2190-04-7	X		8
1-Octadecanamine, N,N-dimethyl-	124-28-7	X		1, 3, 4
1-Octadecene	112-88-9	X		3
1-Octanol	111-87-5	X		1, 4
1-Pentanol	71-41-0	X		8
1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., chlorides, sodium salts	61789-39-7			1

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivs., inner salts	61789-40-0			1, 2, 3, 4
1-Propanaminium, 3-chloro-2-hydroxy-N,N,N-trimethyl-, chloride	3327-22-8	X		8
1-Propanaminium, N-(3-aminopropyl)-2-hydroxy-N,N-dimethyl-3-sulfo-, N-coco acyl derivs., inner salts	68139-30-0			1, 3, 4
1-Propanaminium, N-(carboxymethyl)-N,N-dimethyl-3-[(1-oxooctyl)amino]-, inner salt	73772-46-0			8
1-Propanesulfonic acid	5284-66-2	X		3
1-Propanol	71-23-8	X		1, 2, 4, 5
1-Propanol, zirconium(4+) salt	23519-77-9			1, 4, 8
1-Propene	115-07-1	X		2
1-tert-Butoxy-2-propanol	57018-52-7	X		8
1-Tetradecene	1120-36-1	X		3
1-Tridecanol	112-70-9	X		1, 4
1-Undecanol	112-42-5	X		2
2-(2-Butoxyethoxy)ethanol	112-34-5	X	X	2, 4
2-(2-Ethoxyethoxy)ethanol	111-90-0	X	X	1, 4
2-(2-Ethoxyethoxy)ethyl acetate	112-15-2	X		1, 4
2-(Dibutylamino)ethanol	102-81-8	X		1, 4
2-(Hydroxymethylamino)ethanol	34375-28-5	X		1, 4
2-(Thiocyanomethylthio)benzothiazole	21564-17-0	X	X	2
2,2'-(diazene-1,2-diyl)diethane-1,1-diyl)bis-4,5-dihydro-1H-imidazole dihydrochloride	27776-21-2	X		3
2,2'-(Octadecylimino)diethanol	10213-78-2	X		1
2,2'-[Ethane-1,2-diylbis(oxy)]diethanamine	929-59-9	X		1, 4
2,2'-Azobis(2-amidinopropane) dihydrochloride	2997-92-4	X		1, 4
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	X		1, 2, 3, 4, 6, 7, 8
2,2-Dibromopropanediamide	73003-80-2	X		3
2,4-Hexadienoic acid, potassium salt, (2E,4E)-	24634-61-5	X		3

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
2,6,8-Trimethyl-4-nonanol	123-17-1	X		8
2-Acrylamide - 2-propanesulfonic acid and N,N-dimethylacrylamide copolymer	NOCAS_51252			2
2-Acrylamido -2-methylpropanesulfonic acid copolymer	NOCAS_51255			8
2-Acrylamido-2-methyl-1-propanesulfonic acid	15214-89-8	X		1, 3
2-Amino-2-methylpropan-1-ol	124-68-5	X		8
2-Aminoethanol ester with boric acid (H3BO3) (1:1)	10377-81-8			8
2-Aminoethanol hydrochloride	2002-24-6	X		4, 8
2-Bromo-3-nitrilopropionamide	1113-55-9	X		1, 2, 3, 4, 5
2-Butanone oxime	96-29-7	X		1
2-Butenediamide, (2E)-, N,N'-bis[2-(4,5-dihydro-2-nortall-oil alkyl-1H-imidazol-1-yl)ethyl] derivs.	68442-77-3			3, 8
2-Butoxy-1-propanol	15821-83-7	X		8
2-Butoxyethanol	111-76-2	X	X	1, 2, 3, 4, 6, 7, 8
2-Dodecylbenzenesulfonic acid- n-(2-aminoethyl)ethane-1,2-diamine(1:1)	40139-72-8	X		8
2-Ethoxyethanol	110-80-5	X	X	6
2-Ethoxynaphthalene	93-18-5	X		3
2-Ethyl-1-hexanol	104-76-7	X		1, 2, 3, 4, 5
2-Ethyl-2-hexenal	645-62-5	X		2
2-Ethylhexyl benzoate	5444-75-7	X		4
2-Hydroxyethyl acrylate	818-61-1	X		1, 4
2-Hydroxyethylammonium hydrogen sulphite	13427-63-9	X		1
2-Hydroxy-N,N-bis(2-hydroxyethyl)-N-methylethanaminium chloride	7006-59-9	X		8
2-Mercaptoethanol	60-24-2	X		1, 4
2-Methoxyethanol	109-86-4	X	X	4
2-Methyl-1-propanol	78-83-1	X	X	1, 2, 4
2-Methyl-2,4-pentanediol	107-41-5	X		1, 2, 4

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
2-Methyl-3(2H)-isothiazolone	2682-20-4	X		1, 2, 4
2-Methyl-3-butyn-2-ol	115-19-5	X		3
2-Methylbutane	78-78-4	X		2
2-Methylquinoline hydrochloride	62763-89-7	X		3
2-Phosphono-1,2,4-butanetricarboxylic acid	37971-36-1	X		1, 4
2-Phosphonobutane-1,2,4-tricarboxylic acid, potassium salt (1:x)	93858-78-7	X		1
2-Propanol, aluminum salt	555-31-7			1
2-Propen-1-aminium, N,N-dimethyl-N-2-propenyl-, chloride, homopolymer	26062-79-3			3
2-Propenamide, homopolymer	25038-45-3			8
2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	13533-05-6	X		4
2-Propenoic acid, 2-ethylhexyl ester, polymer with 2-hydroxyethyl 2-propenoate	36089-45-9			8
2-Propenoic acid, 2-methyl-, polymer with 2-propenoic acid, sodium salt	28205-96-1			8
2-Propenoic acid, 2-methyl-, polymer with sodium 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonate (1:1)	136793-29-8			8
2-Propenoic acid, ethyl ester, polymer with ethenyl acetate and 2,5-furandione, hydrolyzed	113221-69-5			4, 8
2-Propenoic acid, ethyl ester, polymer with ethenyl acetate and 2,5-furandione, hydrolyzed, sodium salt	111560-38-4			8
2-Propenoic acid, polymer with 2-propenamide, sodium salt	25987-30-8			3, 4, 8
2-Propenoic acid, polymer with ethene, zinc salt	28208-80-2			8
2-Propenoic acid, polymer with ethenylbenzene	25085-34-1			8
2-Propenoic acid, polymer with sodium ethanesulfonate, peroxydisulfuric acid, disodium salt- initiated, reaction products with tetrasodium ethenylidenebis (phosphonata)	397256-50-7			8
2-Propenoic acid, polymer with sodium phosphinate (1:1), sodium salt	129898-01-7			8

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
2-Propenoic acid, sodium salt (1:1), polymer with sodium 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonate (1:1)	37350-42-8			1
2-Propenoic acid, telomer with sodium 4-ethenylbenzenesulfonate (1:1), sodium 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonate (1:1) and sodium sulfite (1:1), sodium salt	151006-66-5			4
2-Propenoic, polymer with sodium phosphinate	71050-62-9			3, 4
3-(Dimethylamino)propylamine	109-55-7	X		8
3,4,4-Trimethyloxazolidine	75673-43-7	X		8
3,5,7-Triazatricyclo(3.3.1.1 <sup>3,7</sup> )decane, 1-(3-chloro-2-propenyl)-, chloride, (Z)-	51229-78-8	X		3
3,7-Dimethyl-2,6-octadienal	5392-40-5	X		3
3-Hydroxybutanal	107-89-1	X		1, 2, 4
3-Methoxypropylamine	5332-73-0	X		8
3-Phenylprop-2-enal	104-55-2	X		1, 2, 3, 4, 7
4,4-Dimethyloxazolidine	51200-87-4	X		8
4,6-Dimethyl-2-heptanone	19549-80-5	X		8
4-[Abieta-8,11,13-trien-18-yl(3-oxo-3-phenylpropyl)amino]butan-2-one hydrochloride	143106-84-7	X		1, 4
4-Ethyl-1-oct-3-yn-1-ol	5877-42-9	X		1, 2, 3, 4
4-Hydroxy-3-methoxybenzaldehyde	121-33-5	X		3
4-Methoxybenzyl formate	122-91-8	X		3
4-Methoxyphenol	150-76-5	X		4
4-Methyl-2-pentanol	108-11-2	X		1, 4
4-Methyl-2-pentanone	108-10-1	X		5
4-Nonylphenol	104-40-5	X		8
4-Nonylphenol polyethoxylate	68412-54-4			2, 3, 4
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	X		1, 2, 4
Acetaldehyde	75-07-0	X		1, 4
Acetic acid	64-19-7	X		1, 2, 3, 4, 5, 6, 7, 8

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Acetic acid ethenyl ester, polymer with ethenol	25213-24-5			1, 4
Acetic acid, C6-8-branched alkyl esters	90438-79-2	X		4
Acetic acid, hydroxy-, reaction products with triethanolamine	68442-62-6	X		3
Acetic acid, mercapto-, monoammonium salt	5421-46-5	X		2, 8
Acetic anhydride	108-24-7	X		1, 2, 3, 4, 7
Acetone	67-64-1	X	X	1, 3, 4, 6
Acetonitrile, 2,2',2''-nitrilotris-	7327-60-8	X		1, 4
Acetophenone	98-86-2	X	X	1
Acetyltriethyl citrate	77-89-4	X		1, 4
Acrolein	107-02-8	X	X	2
Acrylamide	79-06-1	X	X	1, 2, 3, 4
Acrylamide/ sodium acrylate copolymer	25085-02-3			1, 2, 3, 4, 8
Acrylamide-sodium-2-acrylamido-2-methylpropane sulfonate copolymer	38193-60-1			1, 2, 3, 4
Acrylic acid	79-10-7	X	X	2, 4
Acrylic acid, with sodium-2-acrylamido-2-methyl-1-propanesulfonate and sodium phosphinate	110224-99-2	X		8
Alcohols (C13-C15), ethoxylated	64425-86-1			8
Alcohols, C10-12, ethoxylated	67254-71-1	X		3
Alcohols, C10-14, ethoxylated	66455-15-0			3
Alcohols, C11-14-iso-, C13-rich	68526-86-3	X		3
Alcohols, C11-14-iso-, C13-rich, butoxylated ethoxylated	228414-35-5			1
Alcohols, C11-14-iso-, C13-rich, ethoxylated	78330-21-9	X		3, 4, 8
Alcohols, C12-13, ethoxylated	66455-14-9	X		4
Alcohols, C12-14, ethoxylated	68439-50-9			2, 3, 4, 8
Alcohols, C12-14, ethoxylated propoxylated	68439-51-0	X		1, 3, 4, 8
Alcohols, C12-14-secondary	126950-60-5	X		1, 3, 4
Alcohols, C12-14-secondary, ethoxylated	84133-50-6			3, 4, 8
Alcohols, C12-15, ethoxylated	68131-39-5			3, 4

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Alcohols, C12-16, ethoxylated	68551-12-2	X		3, 4, 8
Alcohols, C14-15, ethoxylated	68951-67-7	X		3, 4, 8
Alcohols, C6-12, ethoxylated	68439-45-2	X		3, 4, 8
Alcohols, C7-9-iso-, C8-rich, ethoxylated	78330-19-5	X		2, 4, 8
Alcohols, C8-10, ethoxylated propoxylated	68603-25-8			3
Alcohols, C9-11, ethoxylated	68439-46-3	X		3, 4
Alcohols, C9-11-iso-, C10-rich, ethoxylated	78330-20-8	X		1, 2, 4, 8
Alkanes C10-16-branched and linear	90622-52-9			4
Alkanes, C10-14	93924-07-3			1
Alkanes, C12-14-iso-	68551-19-9	X		2, 4, 8
Alkanes, C13-16-iso-	68551-20-2	X		1, 4
Alkenes, C>10 .alpha.-	64743-02-8	X		1, 3, 4, 8
Alkenes, C>8	68411-00-7			1
Alkenes, C24-25 alpha-, polymers with maleic anhydride, docosyl esters	68607-07-8			8
Alkyl quaternary ammonium with bentonite	71011-24-0			4
Alkyl* dimethyl ethylbenzyl ammonium chloride *(50%C12, 30%C14, 17%C16, 3%C18)	85409-23-0_1	X		8
Alkyl* dimethyl ethylbenzyl ammonium chloride *(60%C14, 30%C16, 5%C12, 5%C18)	68956-79-6	X		8
Alkylbenzenesulfonate, linear	42615-29-2	X		1, 4, 6
Almandite and pyrope garnet	1302-62-1			1, 4
alpha-[3.5-dimethyl-1-(2-methylpropyl)hexyl]-omega-hydroxy-poly(oxy-1,2-ethandiyl)	60828-78-6			3
alpha-Amylase	9000-90-2			4
alpha-Lactose monohydrate	5989-81-1	X		8
alpha-Terpineol	98-55-5	X		3
Alumina	1344-28-1			1, 2, 4
Aluminatesilicate	1327-36-2			8
Aluminum	7429-90-5		X	1, 4, 6
Aluminum calcium oxide (Al2CaO4)	12042-68-1			2

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Aluminum chloride	7446-70-0			1, 4
Aluminum chloride hydroxide sulfate	39290-78-3			8
Aluminum chloride, basic	1327-41-9			3, 4
Aluminum oxide (Al <sub>2</sub> O <sub>3</sub> )	90669-62-8			8
Aluminum oxide silicate	12068-56-3			1, 2, 4
Aluminum silicate	12141-46-7			1, 2, 4
Aluminum sulfate	10043-01-3			1, 4
Amaranth	915-67-3	X		4
Amides, C8-18 and C18-unsatd., N,N-bis(hydroxyethyl)	68155-07-7			3
Amides, coco, N-[3-(dimethylamino)propyl]	68140-01-2			1, 4
Amides, coco, N-[3-(dimethylamino)propyl], alkylation products with chloroacetic acid, sodium salts	70851-07-9			1, 4
Amides, coco, N-[3-(dimethylamino)propyl], alkylation products with sodium 3-chloro-2-hydroxypropanesulfonate	70851-08-0			8
Amides, coco, N-[3-(dimethylamino)propyl], N-oxides	68155-09-9			1, 3, 4
Amides, from C16-22 fatty acids and diethylenetriamine	68876-82-4			3
Amides, tall-oil fatty, N,N-bis(hydroxyethyl)	68155-20-4			3, 4
Amides, tallow, N-[3-(dimethylamino)propyl],N-oxides	68647-77-8			1, 4
Amine oxides, cocoalkyldimethyl	61788-90-7			8
Amines, C14-18; C16-18-unsaturated, alkyl, ethoxylated	68155-39-5			1
Amines, C8-18 and C18-unsatd. alkyl	68037-94-5			5
Amines, coco alkyl	61788-46-3			4
Amines, coco alkyl, acetates	61790-57-6			1, 4
Amines, coco alkyl, ethoxylated	61791-14-8			8
Amines, coco alkyldimethyl	61788-93-0			8
Amines, dicoco alkyl	61789-76-2			8

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Amines, dicoco alkylmethyl	61788-62-3			8
Amines, ditallow alkyl, acetates	71011-03-5			8
Amines, hydrogenated tallow alkyl, acetates	61790-59-8			4
Amines, N-tallow alkyltrimethylenedi-, ethoxylated	61790-85-0			8
Amines, polyethylenepoly-, ethoxylated, phosphonomethylated	68966-36-9			1, 4
Amines, polyethylenepoly-, reaction products with benzyl chloride	68603-67-8			1
Amines, tallow alkyl	61790-33-8			8
Amines, tallow alkyl, ethoxylated, acetates (salts)	68551-33-7			1, 3, 4
Amines, tallow alkyl, ethoxylated, phosphates	68308-48-5			4
Aminotrimethylene phosphonic acid	6419-19-8	X		1, 4, 8
<i>Ammonia</i>	7664-41-7			1, 2, 3, 4, 7
Ammonium (lauryloxy)polyethoxyethyl sulfate	32612-48-9			4
Ammonium acetate	631-61-8	X		1, 3, 4, 5, 8
Ammonium acrylate	10604-69-0	X		8
Ammonium acrylate-acrylamide polymer	26100-47-0			2, 4, 8
Ammonium bisulfate	7803-63-6			2
Ammonium bisulfite	10192-30-0			1, 2, 3, 4, 7
Ammonium chloride	12125-02-9			1, 2, 3, 4, 5, 6, 8
Ammonium citrate (1:1)	7632-50-0	X		3
Ammonium citrate (2:1)	3012-65-5	X		8
Ammonium dodecyl sulfate	2235-54-3	X		1
Ammonium fluoride	12125-01-8			1, 4
Ammonium hydrogen carbonate	1066-33-7	X		1, 4
Ammonium hydrogen difluoride	1341-49-7			1, 3, 4, 7
Ammonium hydrogen phosphonate	13446-12-3			4
Ammonium hydroxide	1336-21-6			1, 3, 4
Ammonium lactate	515-98-0	X		8

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Ammonium ligninsulfonate	8061-53-8			2
Ammonium nitrate	6484-52-2			1, 2, 3
Ammonium phosphate	7722-76-1		X	1, 4
Ammonium sulfate	7783-20-2			1, 2, 3, 4, 6
Ammonium thiosulfate	7783-18-8			8
Amorphous silica	99439-28-8			1, 7
Anethole	104-46-1	X		3
Aniline	62-53-3	X	X	2, 4
Antimony pentoxide	1314-60-9			1, 4
Antimony trichloride	10025-91-9		X	1, 4
Antimony trioxide	1309-64-4		X	8
<i>Arsenic</i>	7440-38-2		X	4
Ashes, residues	68131-74-8			4
Asphalt, sulfonated, sodium salt	68201-32-1			2
Attapulgate	12174-11-7			2, 3
Aziridine, polymer with 2-methyloxirane	31974-35-3			4, 8
Barium sulfate	7727-43-7			1, 2, 4
Bauxite	1318-16-7			1, 2, 4
Benactyzine hydrochloride	57-37-4	X		8
Bentonite	1302-78-9			1, 2, 4, 6
Bentonite, benzyl(hydrogenated tallow alkyl) dimethylammonium stearate complex	121888-68-4			3, 4
Benzamorf	12068-08-5	X		1, 4
<i>Benzene</i>	71-43-2	X	X	1, 3, 4
Benzene, 1,1'-oxybis-, sec-hexyl derivs., sulfonated, sodium salts	147732-60-3			8
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated	119345-03-8			8
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated, sodium salts	119345-04-9			3, 4, 8
Benzene, C10-16-alkyl derivs.	68648-87-3	X		1

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Benzene, ethenyl-, polymer with 2-methyl-1,3-butadiene, hydrogenated	68648-89-5			8
Benzenemethanaminium, N,N-dimethyl-N-(2-((1-oxo-2-propen-1-yl)oxy)ethyl)-, chloride (1:1), polymer with 2-propenamide	74153-51-8			3
Benzenesulfonic acid	98-11-3	X		2
Benzenesulfonic acid, (1-methylethyl)-,	37953-05-2	X		4
Benzenesulfonic acid, (1-methylethyl)-, ammonium salt	37475-88-0	X		3, 4
Benzenesulfonic acid, (1-methylethyl)-, sodium salt	28348-53-0	X		8
Benzenesulfonic acid, C10-16-alkyl derivs.	68584-22-5		X	1, 4
Benzenesulfonic acid, C10-16-alkyl derivs., compds. with cyclohexylamine	255043-08-4	X		1
Benzenesulfonic acid, C10-16-alkyl derivs., compds. with triethanolamine	68584-25-8	X		8
Benzenesulfonic acid, C10-16-alkyl derivs., potassium salts	68584-27-0	X		1, 4, 8
Benzenesulfonic acid, dodecyl-, branched, compds. with 2-propanamine	90218-35-2	X		4
Benzenesulfonic acid, mono-C10-16 alkyl derivs., compds. with 2-propanamine	68648-81-7			1, 4
Benzenesulfonic acid, mono-C10-16-alkyl derivs., sodium salts	68081-81-2	X		8
Benzoic acid	65-85-0	X	X	1, 4, 7
Benzyl chloride	100-44-7	X	X	1, 2, 4, 8
Benzyltrimethylammonium chloride	139-07-1	X		2, 8
Benzylhexadecyldimethylammonium chloride	122-18-9	X		8
Benzyltrimethylammonium chloride	56-93-9	X		8
Bicine	150-25-4	X		1, 4
Bio-Perge	55965-84-9			8
Bis(1-methylethyl)naphthalenesulfonic acid, cyclohexylamine salt	68425-61-6	X		1
<i>Bis(2-chloroethyl) ether</i>	<i>111-44-4</i>	X	X	8

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Bisphenol A	80-05-7	X	X	4
Bisphenol A/ Epichlorohydrin resin	25068-38-6			1, 2, 4
Bisphenol A/ Novolac epoxy resin	28906-96-9			1, 4
Blast furnace slag	65996-69-2			2, 3
Borax	1303-96-4			1, 2, 3, 4, 6
Boric acid	10043-35-3			1, 2, 3, 4, 6, 7
Boric acid (H3BO3), compd. with 2-aminoethanol (1:x)	26038-87-9			8
Boric oxide	1303-86-2			1, 2, 3, 4
Boron potassium oxide (B4K2O7)	1332-77-0			8
Boron potassium oxide (B4K2O7), tetrahydrate	12045-78-2			8
Boron potassium oxide (B5KO8)	11128-29-3			1
Boron sodium oxide	1330-43-4			1, 2, 4
Boron sodium oxide pentahydrate	12179-04-3			8
Bronopol	52-51-7	X		1, 2, 3, 4, 6
Butane	106-97-8	X		2, 5
Butanedioic acid, sulfo-, 1,4-bis(1,3-dimethylbutyl) ester, sodium salt	2373-38-8	X		1
Butene	25167-67-3	X		8
Butyl glycidyl ether	2426-08-6	X		1, 4
Butyl lactate	138-22-7	X		1, 4
Butyryl trihexyl citrate	82469-79-2	X		8
C.I. Acid Red 1	3734-67-6	X		4
C.I. Acid violet 12, disodium salt	6625-46-3	X		4
C.I. Pigment Red 5	6410-41-9	X		4
C.I. Solvent Red 26	4477-79-6	X		4
C10-16-Alkyldimethylamines oxides	70592-80-2	X		4
C10-C16 ethoxylated alcohol	68002-97-1	X		1, 2, 3, 4, 8
C11-15-Secondary alcohols ethoxylated	68131-40-8			1, 2, 8
C12-14 tert-alkyl ethoxylated amines	73138-27-9	X		3
C8-10 Alcohols	85566-12-7			8

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Calcined bauxite	66402-68-4			2, 8
Calcium aluminate	12042-78-3			2
Calcium bromide	7789-41-5			4
Calcium carbide (CaC <sub>2</sub> )	75-20-7			8
Calcium chloride	10043-52-4			1, 2, 3, 4, 7
Calcium dichloride dihydrate	10035-04-8			1, 4
Calcium dodecylbenzene sulfonate	26264-06-2	X		4
Calcium fluoride	7789-75-5			1, 4
Calcium hydroxide	1305-62-0			1, 2, 3, 4
Calcium hypochlorite	7778-54-3			1, 2, 4
Calcium magnesium hydroxide oxide	58398-71-3			4
Calcium oxide	1305-78-8			1, 2, 4, 7
Calcium peroxide	1305-79-9			1, 3, 4, 8
Calcium sulfate	7778-18-9			1, 2, 4
Calcium sulfate dihydrate	10101-41-4			2
Camphor	76-22-2	X		3
Canola oil	120962-03-0			8
Carbon black	1333-86-4			1, 2, 4
<i>Carbon dioxide</i>	<i>124-38-9</i>	X		<i>1, 3, 4, 6</i>
Carbonic acid calcium salt (1:1)	471-34-1			1, 2, 4
Carbonic acid, dipotassium salt	584-08-7	X		1, 2, 3, 4, 8
Carboxymethyl guar gum, sodium salt	39346-76-4			1, 2, 4
Castor oil	8001-79-4			8
Cedarwood oil	8000-27-9			3
Cellophane	9005-81-6			1, 4
Cellulose	9004-34-6			1, 2, 3, 4
<i>Chloride</i>	<i>16887-00-6</i>			<i>4, 8</i>
<i>Chlorine</i>	<i>7782-50-5</i>		X	2
Chlorine dioxide	10049-04-4		X	1, 2, 3, 4, 8
Choline bicarbonate	78-73-9	X		3, 8

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Choline chloride	67-48-1	X		1, 3, 4, 7, 8
Chromium (III)	16065-83-1		X	2, 6
Chromium (VI)	18540-29-9		X	6
Chromium acetate, basic	39430-51-8			2
Chromium(III) acetate	1066-30-4			1, 2
Citric acid	77-92-9	X		1, 2, 3, 4, 7
Citronella oil	8000-29-1			3
Citronellol	106-22-9	X		3
Citrus extract	94266-47-4			1, 3, 4, 8
Coal, granular	50815-10-6			1, 2, 4
Cobalt(II) acetate	71-48-7			1, 4
Coco-betaine	68424-94-2			3
Coconut oil	8001-31-8			8
Coconut oil acid/Diethanolamine condensate (2:1)	68603-42-9			1
Coconut trimethylammonium chloride	61789-18-2	X		1, 8
Copper	7440-50-8		X	1, 4
Copper sulfate	7758-98-7			1, 4, 8
Copper(I) chloride	7758-89-6			1, 4
Copper(I) iodide	7681-65-4		X	1, 2, 4, 6
Copper(II) chloride	7447-39-4			1, 3, 4
Copper(II) sulfate, pentahydrate	7758-99-8			8
Corn flour	68525-86-0			4
Corn sugar gum	11138-66-2			1, 2, 4
Corundum (Aluminum oxide)	1302-74-5			4, 8
Cottonseed, flour	68308-87-2			2, 4
Coumarin	91-64-5	X		3
Cremophor(R) EL	61791-12-6			1, 3
Cristobalite	14464-46-1			1, 2, 4
Crystalline silica, tridymite	15468-32-3			1, 2, 4

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<b>Chemical name</b>	<b>CASRN</b>	<b>Physico-chemical properties</b>	<b>Selected toxicity reference value</b>	<b>Reference</b>
<i>Cumene</i>	98-82-8	X	X	1, 2, 3, 4
Cupric chloride dihydrate	10125-13-0			1, 4, 7
Cyclohexane	110-82-7	X		1, 7
Cyclohexanol	108-93-0	X		8
Cyclohexanone	108-94-1	X	X	1, 4
Cyclohexylamine sulfate	19834-02-7	X		8
D&C Red 28	18472-87-2	X		4
D&C Red No. 33	3567-66-6	X		8
Daidzein	486-66-8	X		8
Dapsone	80-08-0	X		1, 4
Dazomet	533-74-4	X		1, 2, 3, 4, 7, 8
Decamethylcyclopentasiloxane	541-02-6			8
Decyldimethylamine	1120-24-7	X		3, 4
Deuterium oxide	7789-20-0			8
D-Glucitol	50-70-4	X		1, 3, 4
D-Gluconic acid	526-95-4	X		1, 4
D-Glucopyranoside, methyl	3149-68-6	X		2
D-Glucose	50-99-7	X		1, 4
<i>Di(2-ethylhexyl) phthalate</i>	117-81-7	X	X	1, 4
Diammonium peroxydisulfate	7727-54-0			1, 2, 3, 4, 6, 7, 8
Diatomaceous earth	68855-54-9			2, 4
Diatomaceous earth, calcined	91053-39-3			1, 2, 4
Dibromoacetonitrile	3252-43-5	X		1, 2, 3, 4, 8
Dicalcium silicate	10034-77-2			1, 2, 4
<i>Dichloromethane</i>	75-09-2	X	X	8
Didecyldimethylammonium chloride	7173-51-5	X	X	1, 2, 4, 8
Diethanolamine	111-42-2	X		1, 2, 3, 4, 6
Diethylbenzene	25340-17-4	X		1, 3, 4
Diethylene glycol	111-46-6	X		1, 2, 3, 4, 7

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Diethylene glycol monomethyl ether	111-77-3	X		1, 2, 4
Diethylenetriamine	111-40-0	X		1, 2, 4, 5
Diethylenetriamine reaction product with fatty acid dimers	68647-57-4			2
Diisobutyl ketone	108-83-8	X		8
Diisopropanolamine	110-97-4	X		8
Diisopropyl naphthalene	38640-62-9	X		3, 4
Dimethyl adipate	627-93-0	X		8
Dimethyl glutarate	1119-40-0	X		1, 4
Dimethyl polysiloxane	63148-62-9			1, 2, 4
Dimethyl succinate	106-65-0	X		8
Dimethylaminoethanol	108-01-0	X		2, 4
Dimethyldiallylammonium chloride	7398-69-8	X		3, 4
Diphenyl oxide	101-84-8	X		3
Dipotassium monohydrogen phosphate	7758-11-4			5
Dipropylene glycol	25265-71-8	X		1, 3, 4
Di-sec-butylphenol	31291-60-8	X		1
Disodium dodecyl(sulphonatophenoxy) benzenesulphonate	28519-02-0	X		1
Disodium ethylenediaminediacetate	38011-25-5	X		1, 4
Disodium ethylenediaminetetraacetate dihydrate	6381-92-6	X		1
Disodium octaborate	12008-41-2			4, 8
Disodium octaborate tetrahydrate	12280-03-4			1, 4
Disodium sulfide	1313-82-2			8
Distillates, petroleum, catalytic reformer fractionator residue, low-boiling	68477-31-6			1, 4
Distillates, petroleum, heavy arom.	67891-79-6			1, 4
Distillates, petroleum, hydrodesulfurized light catalytic cracked	68333-25-5			1
Distillates, petroleum, hydrodesulfurized middle	64742-80-9			1

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Distillates, petroleum, hydrotreated heavy naphthenic	64742-52-5			1, 2, 3, 4
Distillates, petroleum, hydrotreated heavy paraffinic	64742-54-7			1, 2, 4
Distillates, petroleum, hydrotreated light	64742-47-8			1, 2, 3, 4, 5, 7, 8
Distillates, petroleum, hydrotreated light naphthenic	64742-53-6			1, 2, 8
Distillates, petroleum, hydrotreated light paraffinic	64742-55-8			8
Distillates, petroleum, hydrotreated middle	64742-46-7			1, 2, 3, 4, 8
Distillates, petroleum, light catalytic cracked	64741-59-9			1, 4
Distillates, petroleum, light hydrocracked	64741-77-1			3
Distillates, petroleum, solvent-dewaxed heavy paraffinic	64742-65-0			1
Distillates, petroleum, solvent-refined heavy naphthenic	64741-96-4			1, 4
Distillates, petroleum, steam-cracked	64742-91-2			1, 4
Distillates, petroleum, straight-run middle	64741-44-2			1, 2, 4
Distillates, petroleum, sweetened middle	64741-86-2			1, 4
Ditallow alkyl ethoxylated amines	71011-04-6			3
D-Lactic acid	10326-41-7	X		1, 4
D-Limonene	5989-27-5	X	X	1, 3, 4, 5, 7, 8
Docusate sodium	577-11-7	X		1
Dodecamethylcyclohexasiloxane	540-97-6			8
Dodecane	112-40-3	X		8
Dodecylbenzene	123-01-3	X		3, 4
Dodecylbenzenesulfonic acid	27176-87-0	X	X	2, 3, 4, 8
Dodecylbenzenesulfonic acid, monoethanolamine salt	26836-07-7	X		1, 4
Edifas B	9004-32-4			2, 3, 4
EDTA, copper salt	12276-01-6			1, 5, 6
Endo-1,4-.beta.-mannanase	37288-54-3			3, 8

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Epichlorohydrin	106-89-8	X	X	1, 4, 8
Epoxy resin	25085-99-8			1, 4, 8
Erucic amidopropyl dimethyl betaine	149879-98-1			1, 3
Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride	44992-01-0	X		3
Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-,chloride, polymer with 2-propenamamide	69418-26-4			1, 3, 4
Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propen-1-yl)oxy]-, chloride (1:1), polymer with 2-propenamamide	35429-19-7			8
Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, methyl sulfate, homopolymer	27103-90-8			8
Ethane	74-84-0	X		2, 5
Ethanol	64-17-5	X		1, 2, 3, 4, 5, 6, 8
Ethanol, 2,2',2''-nitrilotris-, tris(dihydrogen phosphate) (ester), sodium salt	68171-29-9	X		4
Ethanol, 2,2'-iminobis-, N-coco alkyl derivs., N-oxides	61791-47-7			1
Ethanol, 2,2'-iminobis-, N-tallow alkyl derivs.	61791-44-4			1
Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues	68909-77-3			4, 8
Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues, acetates (salts)	68877-16-7			4
Ethanol, 2,2'-oxybis-, reaction products with ammonia, morpholine derivs. residues, reaction products with sulfur dioxide	102424-23-7			4
Ethanol, 2-[2-[2-(tridecyloxy)ethoxy]ethoxy]-, hydrogen sulfate, sodium salt	25446-78-0	X		1, 4
Ethanol, 2-amino-, polymer with formaldehyde	34411-42-2			4
Ethanol, 2-amino-, reaction products with ammonia, by-products from, phosphonomethylated	68649-44-5			4

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Ethanolamine	141-43-5	X		1, 2, 3, 4, 6
Ethoxylated dodecyl alcohol	9002-92-0	X		4
Ethoxylated hydrogenated tallow alkylamines	61790-82-7			4
Ethoxylated, propoxylated trimethylolpropane	52624-57-4			3
Ethyl acetate	141-78-6	X	X	1, 4, 7
Ethyl acetoacetate	141-97-9	X		1, 4
Ethyl benzoate	93-89-0	X		3
Ethyl lactate	97-64-3	X		3
Ethyl salicylate	118-61-6	X		3
<i>Ethylbenzene</i>	<i>100-41-4</i>	X	X	1, 2, 3, 4, 7
Ethylcellulose	9004-57-3			2
Ethylene	74-85-1	X		8
<i>Ethylene glycol</i>	<i>107-21-1</i>	X	X	1, 2, 3, 4, 6, 7, 8
Ethylene oxide	75-21-8	X	X	1, 2, 3, 4
Ethylenediamine	107-15-3	X	X	2, 4
Ethylenediaminetetraacetic acid	60-00-4	X		1, 2, 4
Ethylenediaminetetraacetic acid tetrasodium salt	64-02-8	X		1, 2, 3, 4
Ethylenediaminetetraacetic acid, diammonium copper salt	67989-88-2			4
Ethylenediaminetetraacetic acid, disodium salt	139-33-3	X		1, 3, 4, 8
Ethyne	74-86-2	X		7
Fats and Glyceridic oils, vegetable, hydrogenated	68334-28-1			8
Fatty acid, tall oil, hexa esters with sorbitol, ethoxylated	61790-90-7			1, 4
Fatty acids, C 8-18 and C18-unsaturated compounds with diethanolamine	68604-35-3			3
Fatty acids, C14-18 and C16-18-unsatd., distn. residues	70321-73-2			2
Fatty acids, C18-unsatd., dimers	61788-89-4	X		2

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Fatty acids, C18-unsatd., dimers, compds. with ethoxylated tall-oil fatty acid-polyethylenepolyamine reaction products	68132-59-2			8
Fatty acids, C18-unsatd., dimers, ethoxylated propoxylated	68308-89-4			8
Fatty acids, coco, ethoxylated	61791-29-5			3
Fatty acids, coco, reaction products with diethylenetriamine and soya fatty acids, ethoxylated, chloromethane-quaternized	68604-75-1			8
Fatty acids, coco, reaction products with ethanolamine, ethoxylated	61791-08-0			3
Fatty acids, tall oil, reaction products with acetophenone, formaldehyde and thiourea	68188-40-9			3
Fatty acids, tall-oil	61790-12-3			1, 2, 3, 4
Fatty acids, tall-oil, reaction products with diethylenetriamine	61790-69-0			1, 4
Fatty acids, tall-oil, reaction products with diethylenetriamine, maleic anhydride, tetraethylenepentamine and triethylenetetramine	68990-47-6			8
Fatty acids, tallow, sodium salts	8052-48-0			1, 3
Fatty acids, vegetable-oil, reaction products with diethylenetriamine	68153-72-0			3
Fatty quaternary ammonium chloride	61789-68-2			1, 4
FD&C Blue no. 1	3844-45-9	X		1, 4
FD&C Yellow 5	1934-21-0	X		8
FD&C Yellow 6	2783-94-0	X		8
Ferric chloride	7705-08-0			1, 3, 4
Ferric sulfate	10028-22-5			1, 4
Ferrous sulfate monohydrate	17375-41-6			2
Ferumoxytol	1309-38-2			8
Fiberglass	65997-17-3			2, 3, 4
Formaldehyde	50-00-0	X	X	1, 2, 3, 4

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Formaldehyde polymer with 4,1,1-(dimethylethyl)phenol and methyloxirane	29316-47-0			3
Formaldehyde polymer with methyl oxirane, 4-nonylphenol and oxirane	63428-92-2			4, 8
Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane and oxirane	30704-64-4			1, 2, 4, 8
Formaldehyde, polymer with 4-(1,1-dimethylethyl)phenol, 2-methyloxirane, 4-nonylphenol and oxirane	68188-99-8			8
Formaldehyde, polymer with 4-nonylphenol and oxirane	30846-35-6			1, 4
Formaldehyde, polymer with 4-nonylphenol and phenol	40404-63-5			8
Formaldehyde, polymer with ammonia and phenol	35297-54-2			1, 4
Formaldehyde, polymer with bisphenol A	25085-75-0			4
Formaldehyde, polymer with N1-(2-aminoethyl)-1,2-ethanediamine, benzylated	70750-07-1			8
Formaldehyde, polymer with nonylphenol and oxirane	55845-06-2			4
Formaldehyde, polymers with branched 4-nonylphenol, oxirane and 2-methyloxirane	153795-76-7			1 3
Formaldehyde/ amine	50-00-0_3			1, 2, 3, 4
Formamide	75-12-7	X		1, 2, 3, 4
<i>Formic acid</i>	<i>64-18-6</i>	X	X	<i>1, 2, 3, 4, 6, 7</i>
Formic acid, potassium salt	590-29-4	X		1, 3, 4
Frits, chemicals	65997-18-4			8
Fuel oil, no. 2	68476-30-2			1, 2
Fuels, diesel	68334-30-5			2
Fuels, diesel, no. 2	68476-34-6			2, 4, 8
Fuller's earth	8031-18-3			2
Fumaric acid	110-17-8	X		1, 2, 3, 4, 6
Fumes, silica	69012-64-2			8

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Furfural	98-01-1	X	X	1, 4
Furfuryl alcohol	98-00-0	X		1, 4
Galantamine hydrobromide	69353-21-5	X		8
Gas oils, petroleum, straight-run	64741-43-1			1, 4
Gelatin	9000-70-8			1, 4
Gilsonite	12002-43-6			1, 2, 4
Gluconic acid	133-42-6	X		7
Glutaraldehyde	111-30-8	X		1, 2, 3, 4, 7
Glycerides, C14-18 and C16-18-unsatd. mono- and di-	67701-32-0			8
Glycerol	56-81-5	X		1, 2, 3, 4, 5
Glycine, N-(carboxymethyl)-N-(2-hydroxyethyl)-, disodium salt	135-37-5	X		1
Glycine, N-(hydroxymethyl)-, monosodium salt	70161-44-3	X		8
Glycine, N,N-bis(carboxymethyl)-, trisodium salt	5064-31-3	X		1, 2, 3, 4
Glycine, N-[2-[bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyethyl)-, trisodium salt	139-89-9	X		1
Glycolic acid	79-14-1	X		1, 3, 4
Glycolic acid sodium salt	2836-32-0	X		1, 3, 4
Glyoxal	107-22-2	X	X	1, 2, 4
Glyoxylic acid	298-12-4	X		1
Goethite (Fe(OH)O)	1310-14-1			8
Guar gum	9000-30-0			1, 2, 3, 4, 7, 8
Guar gum, carboxymethyl 2-hydroxypropyl ether, sodium salt	68130-15-4			1, 2, 3, 4, 7
Gypsum (Ca(SO <sub>4</sub> ).2H <sub>2</sub> O)	13397-24-5			2, 4
Hematite	1317-60-8			1, 2, 4
Hemicellulase	9012-54-8			1, 2, 3, 4, 5
Hemicellulase enzyme concentrate	9025-56-3			3, 4
Heptane	142-82-5	X		1, 2
Heptene, hydroformylation products, high-boiling	68526-88-5			1, 4

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Hexadecyltrimethylammonium bromide	57-09-0	X		1
Hexane	110-54-3	X	X	5
Hexanedioic acid	124-04-9	X	X	1, 2, 4, 6
Humic acids, commercial grade	1415-93-6			2
Hydrazine	302-01-2		X	8
Hydrocarbons, terpene processing by-products	68956-56-9			1, 3, 4
Hydrochloric acid	7647-01-0			1, 2, 3, 4, 5, 6, 7, 8
Hydrogen fluoride	7664-39-3			1, 2, 4
Hydrogen peroxide	7722-84-1			1, 3, 4
Hydrogen sulfide	7783-06-4			1, 2
Hydroxyethylcellulose	9004-62-0			1, 2, 3, 4
Hydroxylamine hydrochloride	5470-11-1			1, 3, 4
Hydroxylamine sulfate (2:1)	10039-54-0			4
Hydroxypropyl cellulose	9004-64-2			2, 4
Hydroxypropyl guar gum	39421-75-5			1, 3, 4, 5, 6, 8
Hydroxyvaleric acid	1619-16-5	X		8
Hypochlorous acid	7790-92-3			8
Illite	12173-60-3			8
Ilmenite (FeTiO <sub>3</sub> ), conc.	98072-94-7			8
Indole	120-72-9	X		2
Inulin, carboxymethyl ether, sodium salt	430439-54-6			1, 4
Iridium oxide	12030-49-8			8
<i>Iron</i>	7439-89-6		X	2, 4
Iron oxide	1332-37-2			1, 4
Iron oxide (Fe <sub>3</sub> O <sub>4</sub> )	1317-61-9			4
Iron(II) sulfate	7720-78-7			2
Iron(II) sulfate heptahydrate	7782-63-0			1, 2, 3, 4
Iron(III) oxide	1309-37-1			1, 2, 4
Isoascorbic acid	89-65-6	X		1, 3, 4

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Isobutane	75-28-5	X		2
Isobutene	115-11-7	X		8
Isooctanol	26952-21-6	X		1, 4, 5
Isopentyl alcohol	123-51-3	X		1, 4
<i>Isopropanol</i>	<i>67-63-0</i>	X		1, 2, 3, 4, 6, 7
Isopropanolamine dodecylbenzene	42504-46-1	X		1, 3, 4
Isopropylamine	75-31-0	X		1, 4
Isoquinoline	119-65-3	X		8
Isoquinoline, reaction products with benzyl chloride and quinoline	68909-80-8	X		3
Isoquinolinium, 2-(phenylmethyl)-, chloride	35674-56-7	X		3
Isotridecanol, ethoxylated	9043-30-5			1, 3, 4, 8
Kaolin	1332-58-7			1, 2, 4
Kerosine, petroleum, hydrodesulfurized	64742-81-0			1, 2, 4
Kieselguhr	61790-53-2			1, 2, 4
Kyanite	1302-76-7			1, 2, 4
Lactic acid	50-21-5	X		1, 4, 8
Lactose	63-42-3	X		3
Latex 2000 TM	9003-55-8			2, 4
Lauryl hydroxysultaine	13197-76-7	X		1
Lavandula hybrida abrial herb oil	8022-15-9			3
L-Dilactide	4511-42-6	X		1, 4
<i>Lead</i>	<i>7439-92-1</i>		X	1, 4
Lecithin	8002-43-5			4
L-Glutamic acid	56-86-0	X		8
Lignite	129521-66-0			2
Lignosulfuric acid	8062-15-5			2
Ligroine	8032-32-4			8
Limestone	1317-65-3			1, 2, 3, 4
Linseed oil	8001-26-1			8

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L-Lactic acid	79-33-4	X		1, 4, 8
Magnesium carbonate (1:1)	7757-69-9			8
Magnesium carbonate (1:x)	546-93-0			1, 3, 4
Magnesium chloride	7786-30-3			1, 2, 4
Magnesium chloride hexahydrate	7791-18-6			4
Magnesium hydroxide	1309-42-8			1, 4
Magnesium iron silicate	19086-72-7			1, 4
Magnesium nitrate	10377-60-3			1, 2, 4
Magnesium oxide	1309-48-4			1, 2, 3, 4
Magnesium peroxide	14452-57-4			1, 4
Magnesium phosphide	12057-74-8			1
Magnesium silicate	1343-88-0			1, 4
Magnesium sulfate	7487-88-9			8
Maleic acid homopolymer	26099-09-2			8
Methanamine-N-methyl polymer with chloromethyl oxirane	25988-97-0			4
Methane	74-82-8	X		2, 5
<i>Methanol</i>	67-56-1	X	X	1, 2, 3, 4, 5, 6, 7, 8
Methenamine	100-97-0	X		1, 2, 4
Methoxyacetic acid	625-45-6	X		8
Methyl cellulose	9004-67-5			8
Methyl salicylate	119-36-8	X		1, 2, 3, 4, 7
Methyl vinyl ketone	78-94-4	X		1, 4
Methylcyclohexane	108-87-2	X		1
Methylene bis(thiocyanate)	6317-18-6	X		2
Methylenebis(5-methyloxazolidine)	66204-44-2	X		2
Methyloxirane polymer with oxirane, mono (nonylphenol) ether, branched	68891-11-2			3
Mica	12001-26-2			1, 2, 4, 6
Mineral oil - includes paraffin oil	8012-95-1		X	4, 8

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Mineral spirits	64475-85-0			2
Mono- and di- potassium salts of phosphorous acid	13492-26-7			8
Montmorillonite	1318-93-0			2
Morpholine	110-91-8	X		1, 2, 4
Morpholinium, 4-ethyl-4-hexadecyl-, ethyl sulfate	78-21-7	X		8
MT 6	76-31-3			8
Mullite	1302-93-8			1,2, 4, 8
N-(2-Acryloyloxyethyl)-N-benzyl-N,N-dimethylammonium chloride	46830-22-2	X		3
N-(3-Chloroallyl)hexaminium chloride	4080-31-3	X		8
N,N,N-Trimethyl-2[1-oxo-2-propenyl]oxy ethanaminium chloride, homopolymer	54076-97-0			3
N,N,N-Trimethyl-3-((1-oxooctadecyl)amino)-1-propanaminium methyl sulfate	19277-88-4	X		1
N,N,N-Trimethyloctadecan-1-aminium chloride	112-03-8	X		1, 3, 4
N,N'-Dibutylthiourea	109-46-6	X		1, 4
N,N-Dimethyldecylamine oxide	2605-79-0	X		1, 3, 4
N,N-Dimethylformamide	68-12-2	X	X	1, 2, 4, 5, 8
N,N-Dimethylmethanamine hydrochloride	593-81-7	X		1, 4, 5, 7
N,N-Dimethyl-methanamine-N-oxide	1184-78-7	X		3
N,N-dimethyloctadecylamine hydrochloride	1613-17-8	X		1, 4
N,N'-Methylenebisacrylamide	110-26-9	X		1, 4
Naphtha, petroleum, heavy catalytic reformed	64741-68-0			1, 2, 3, 4
Naphtha, petroleum, hydrotreated heavy	64742-48-9			1, 2, 3, 4, 8
<i>Naphthalene</i>	91-20-3	X	X	1, 2, 3, 4, 5, 7
Naphthalenesulfonic acid, bis(1-methylethyl)-	28757-00-8	X		1, 3, 4
Naphthalenesulfonic acid, polymer with formaldehyde, sodium salt	9084-06-4			2
Naphthalenesulphonic acid, bis (1-methylethyl)-methyl derivatives	99811-86-6	X		1

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Naphthenic acid ethoxylate	68410-62-8	X		4
Navy fuels JP-5	8008-20-6_2			1, 2, 3, 4, 8
Nickel sulfate	7786-81-4			2
Nickel(II) sulfate hexahydrate	10101-97-0			1, 4
Nitriles, tallow, hydrogenated	61790-29-2			4
Nitrilotriacetamide	4862-18-4	X		1, 4, 7
Nitrilotriacetic acid	139-13-9	X	X	1, 4
Nitrilotriacetic acid trisodium monohydrate	18662-53-8	X	X	1, 4
Nitrogen	7727-37-9			1, 2, 3, 4, 6
N-Methyl-2-pyrrolidone	872-50-4	X	X	1, 4
N-Methyldiethanolamine	105-59-9	X		2, 4, 8
N-Methylethanolamine	109-83-1	X		4
N-Methyl-N-hydroxyethyl-N-hydroxyethoxyethylamine	68213-98-9	X		4
N-Oleyl diethanolamide	13127-82-7	X		1, 4
Nonyl nonoxynol-10	9014-93-1			4
Nonylphenol (mixed)	25154-52-3			1, 4
Octamethylcyclotetrasiloxane	556-67-2			8
Octoxynol-9	9036-19-5			1, 2, 3, 4, 8
Oil of eucalyptus	8000-48-4			3
Oil of lemongrass	8007-02-1			3
Oil of rosemary	8000-25-7			3
Oleic acid	112-80-1	X		2, 4
Olivine-group minerals	1317-71-1			4
Orange terpenes	8028-48-6			4
Oxirane, 2-methyl-, polymer with oxirane, ether with (chloromethyl) oxirane polymer with 4,4'-(1-methylidene) bis[phenol]	68036-95-3			8
Oxirane, 2-methyl-, polymer with oxirane, mono(2-ethylhexyl) ether	64366-70-7			8
Oxirane, 2-methyl-, polymer with oxirane, monodecyl ether	37251-67-5			8

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Oxirane, methyl-, polymer with oxirane, mono-C10-16-alkyl ethers, phosphates	68649-29-6			1, 4
Oxygen	7782-44-7			4
Ozone	10028-15-6			8
Paraffin waxes and Hydrocarbon waxes	8002-74-2			1
Paraformaldehyde	30525-89-4			2
PEG-10 Hydrogenated tallow amine	61791-26-2			1, 3
Pentaethylenehexamine	4067-16-7	X		4
Pentane	109-66-0	X		2, 5
Pentyl acetate	628-63-7	X		3
Pentyl butyrate	540-18-1	X		3
Peracetic acid	79-21-0	X		8
Perboric acid, sodium salt, monohydrate	10332-33-9			1, 8
Perlite	93763-70-3			4
Petrolatum, petroleum, oxidized	64743-01-7			3
Petroleum	8002-05-9			1, 2
Petroleum distillate hydrotreated light	6742-47-8			8
<i>Phenanthrene</i>	<i>85-01-8</i>	X		6
<i>Phenol</i>	<i>108-95-2</i>	X	X	1, 2, 4
Phenol, 4,4'-(1-methylethylidene)bis-, polymer with 2-(chloromethyl)oxirane, 2-methyloxirane and oxirane	68123-18-2			8
Phenol-formaldehyde resin	9003-35-4			1, 2, 4, 7
Phosphine	7803-51-2		X	1, 4
Phosphonic acid	13598-36-2			1, 4
Phosphonic acid (dimethylamino(methylene))	29712-30-9	X		1
Phosphonic acid, (((2-[(2-hydroxyethyl)(phosphonomethyl)amino]ethyl)imino]bis(methylene))bis-, compd. with 2-aminoethanol	129828-36-0	X		1
Phosphonic acid, (1-hydroxyethylidene)bis-, potassium salt	67953-76-8	X		4

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Phosphonic acid, (1-hydroxyethylidene)bis-, tetrasodium salt	3794-83-0	X		1, 4
Phosphonic acid, [[[phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]]tetrakis-	15827-60-8	X		1, 2, 4
Phosphonic acid, [[[phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]]tetrakis-, ammonium salt (1:x)	70714-66-8	X		3
Phosphonic acid, [[[phosphonomethyl)imino]bis[2,1-ethanediylnitrilobis(methylene)]]]tetrakis-, sodium salt	22042-96-2	X		3
Phosphonic acid, [[[phosphonomethyl)imino]bis[6,1-hexanediylnitrilobis(methylene)]]]tetrakis-	34690-00-1	X		1, 4, 8
Phosphoric acid	7664-38-2		X	1, 2, 4
Phosphoric acid, aluminium sodium salt	7785-88-8		X	1, 2
Phosphoric acid, ammonium salt (1:3)	10361-65-6			8
Phosphoric acid, diammonium salt	7783-28-0		X	2
Phosphoric acid, mixed decyl and Et and octyl esters	68412-60-2			1
Phosphorous acid	10294-56-1			1
Phthalic anhydride	85-44-9	X	X	1, 4
Pine oils	8002-09-3			1, 2, 4
Pluronic F-127	9003-11-6			1, 3, 4, 8
Policapram (Nylon 6)	25038-54-4			1, 4
Poly (acrylamide-co-acrylic acid), partial sodium salt	62649-23-4			3, 4
Poly(acrylamide-co-acrylic acid)	9003-06-9			4, 8
Poly(lactide)	26680-10-4			1
Poly(oxy-1,2-ethanediy), .alpha.-(nonylphenyl)-.omega.-hydroxy-, phosphate	51811-79-1			1, 4
Poly(oxy-1,2-ethanediy), .alpha.-(octylphenyl)-.omega.-hydroxy-, branched	68987-90-6	X		1, 4

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Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[[(9Z)-9-octadecenylimino]di-2,1-ethanediyl]bis[.omega.-hydroxy-	26635-93-8			1, 4
Poly(oxy-1,2-ethanediyl), .alpha.-[(9Z)-1-oxo-9-octadecenyl]-.omega.-hydroxy-	9004-96-0			8
Poly(oxy-1,2-ethanediyl), .alpha.-hydro-.omega.-hydroxy-, mono-C10-14-alkyl ethers, phosphates	68585-36-4			8
Poly(oxy-1,2-ethanediyl), .alpha.-hydro-.omega.-hydroxy-, mono-C8-10-alkyl ethers, phosphates	68130-47-2			8
Poly(oxy-1,2-ethanediyl), .alpha.-isodecyl-.omega.-hydroxy-	61827-42-7			8
Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C10-16-alkyl ethers, sodium salts	68585-34-2			8
Poly(oxy-1,2-ethanediyl), .alpha.-sulfo-.omega.-hydroxy-, C12-14-alkyl ethers, sodium salts	68891-38-3			1, 4
Poly(oxy-1,2-ethanediyl), alpha-(2,3,4,5-tetramethylnonyl)-omega-hydroxy	68015-67-8			1
Poly(oxy-1,2-ethanediyl), alpha-(nonylphenyl)-omega-hydroxy-, branched, phosphates	68412-53-3			1
Poly(oxy-1,2-ethanediyl), alpha-hexyl-omega-hydroxy	31726-34-8			3, 8
Poly(oxy-1,2-ethanediyl), alpha-hydro-omega-hydroxy-, (9Z)-9-octadecenoate	56449-46-8			3
Poly(oxy-1,2-ethanediyl), alpha-hydro-omega-hydroxy-, ether with alpha-fluoro-omega-(2-hydroxyethyl)poly(difluoromethylene) (1:1)	65545-80-4			1
Poly(oxy-1,2-ethanediyl), alpha-hydro-omega-hydroxy-, ether with D-glucitol (2:1), tetra-(9Z)-9-octadecenoate	61723-83-9			8
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(decyloxy)-, ammonium salt (1:1)	52286-19-8			4
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(hexyloxy)-, ammonium salt (1:1)	63428-86-4			1, 3, 4
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(hexyloxy)-, C6-10-alkyl ethers, ammonium salts	68037-05-8			3, 4

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Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega--(nonylphenoxy)-	9081-17-8			4
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-(octyloxy)-, ammonium salt (1:1)	52286-18-7			4
Poly(oxy-1,2-ethanediyl), alpha-sulfo-omega-hydroxy-, C10-12-alkyl ethers, ammonium salts	68890-88-0			8
Poly(oxy-1,2-ethanediyl), alpha-tridecyl-omega-hydroxy-	24938-91-8			1, 3, 4
Poly(oxy-1,2-ethanediyl), alpha-undecyl-omega-hydroxy-, branched and linear	127036-24-2			1
Poly-(oxy-1,2-ethanediyl)-alpha-undecyl-omega-hydroxy	34398-01-1			1, 3, 4, 8
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy branched	127087-87-0			1, 2, 3, 4
Poly(sodium-p-styrenesulfonate)	25704-18-1			1,4
Poly(tetrafluoroethylene)	9002-84-0			8
Poly[imino(1,6-dioxo-1,6-hexanediyl)imino-1,6-hexanediyl]	32131-17-2			2
Polyacrylamide	9003-05-8			1, 2, 4, 6
Polyacrylate/ polyacrylamide blend	NOCAS_51256			2
Polyacrylic acid, sodium bisulfite terminated	66019-18-9			3
Polyethylene glycol	25322-68-3			1, 2, 3, 4, 7, 8
Polyethylene glycol (9Z)-9-octadecenyl ether	9004-98-2			8
Polyethylene glycol ester with tall oil fatty acid	68187-85-9			1
Polyethylene glycol monobutyl ether	9004-77-7			1, 4
Polyethylene glycol mono-C8-10-alkyl ether sulfate ammonium	68891-29-2			1, 3, 4
Polyethylene glycol nonylphenyl ether	9016-45-9			1, 2, 3, 4, 8
Polyethylene glycol tridecyl ether phosphate	9046-01-9			1, 3, 4
Polyethyleneimine	9002-98-6			4
Polyglycerol	25618-55-7			2
Poly-L-aspartic acid sodium salt	34345-47-6			8
Polyoxyethylene sorbitan trioleate	9005-70-3			3

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Polyoxyethylene(10)nonylphenyl ether	26027-38-3			1, 2, 3, 4, 8
Polyoxyl 15 hydroxystearate	70142-34-6			8
Polyoxypropylenediamine	9046-10-0			1
Polyphosphoric acids, esters with triethanolamine, sodium salts	68131-72-6			1
Polyphosphoric acids, sodium salts	68915-31-1		X	1, 4
Polypropylene glycol	25322-69-4			1, 2, 4
Polypropylene glycol glycerol triether, epichlorohydrin, bisphenol A polymer	68683-13-6			1
Polyquaternium 5	26006-22-4			1, 4
Polysorbate 20	9005-64-5			8
Polysorbate 60	9005-67-8			3, 4
Polysorbate 80	9005-65-6			3, 4
Polyvinyl acetate copolymer	9003-20-7			2
Polyvinyl acetate, partially hydrolyzed	304443-60-5			8
Polyvinyl alcohol	9002-89-5			1, 2, 4
Polyvinyl alcohol/polyvinyl acetate copolymer	NOCAS_50147			2
Polyvinylidene chloride	9002-85-1			8
Polyvinylpyrrolidone	9003-39-8			8
Portland cement	65997-15-1			2, 4
Potassium acetate	127-08-2	X		1, 3, 4
Potassium aluminum silicate	1327-44-2			5
Potassium antimonate	29638-69-5			1, 4
Potassium bisulfate	7646-93-7			8
Potassium borate	12712-38-8			3
Potassium borate (1:x)	20786-60-1			1, 3
Potassium carbonate sesquihydrate	6381-79-9			5
Potassium chloride	7447-40-7			1, 2, 3, 4, 5, 6, 7
Potassium dichromate	7778-50-9			4
Potassium hydroxide	1310-58-3			1, 2, 3, 4, 6

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Potassium iodide	7681-11-0		X	1, 4
Potassium metaborate	13709-94-9			1, 2, 3, 4, 8
Potassium oleate	143-18-0	X		4
Potassium oxide	12136-45-7			1, 4
Potassium persulfate	7727-21-1			1, 2, 4
Potassium phosphate, tribasic	7778-53-2		X	8
Potassium sulfate	7778-80-5			2
Propane	74-98-6	X		2, 5
Propanol, 1(or 2)-(2-methoxymethylethoxy)-	34590-94-8	X		1, 2, 3, 4
Propargyl alcohol	107-19-7	X	X	1, 2, 3, 4, 5, 6, 7, 8
Propylene carbonate	108-32-7	X		1, 4
Propylene pentamer	15220-87-8	X		1
p-Xylene	106-42-3	X		1, 4
Pyridine, alkyl derivs.	68391-11-7			1, 4
Pyridinium, 1-(phenylmethyl)-, alkyl derivs., chlorides	100765-57-9			4, 8
Pyridinium, 1-(phenylmethyl)-, C7-8-alkyl derivs., chlorides	70914-44-2			6
Pyrimidine	289-95-2	X		2
Pyrrrole	109-97-7	X		2
Quartz-alpha (SiO <sub>2</sub> )	14808-60-7			1, 2, 3, 4, 5, 6, 8
Quaternary ammonium compounds (2-ethylhexyl) hydrogenated tallow alkyl)dimethyl, methyl sulfates	308074-31-9			8
Quaternary ammonium compounds, (oxydi-2,1-ethanediyl)bis[coco alkyldimethyl, dichlorides	68607-28-3			2, 3, 4, 8
Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, bis(hydrogenated tallow alkyl)dimethylammonium salt with bentonite	71011-25-1			8

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Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with bentonite	68153-30-0			2, 5, 6
Quaternary ammonium compounds, benzyl-C10-16-alkyldimethyl, chlorides	68989-00-4			1, 4
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1		X	1, 2, 4, 8
Quaternary ammonium compounds, benzyl-C12-18-alkyldimethyl, chlorides	68391-01-5			8
Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite	68953-58-2			2, 3, 4, 8
Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with hectorite	71011-27-3			2
Quaternary ammonium compounds, di-C8-10-alkyldimethyl, chlorides	68424-95-3	X		2
Quaternary ammonium compounds, dicoco alkyldimethyl, chlorides	61789-77-3			1
Quaternary ammonium compounds, pentamethyltallow alkyltrimethylenedi-, dichlorides	68607-29-4			4
Quaternary ammonium compounds, trimethyltallow alkyl, chlorides	8030-78-2			1, 4
Quinaldine	91-63-4	X		8
Quinoline	91-22-5	X	X	2, 4
Raffinates (petroleum)	68514-29-4			5
Raffinates, petroleum, sorption process	64741-85-1			1, 2, 4, 8
Residual oils, petroleum, solvent-refined	64742-01-4			5
Residues, petroleum, catalytic reformer fractionator	64741-67-9			1, 4, 8
Rhodamine B	81-88-9	X		4
Rosin	8050-09-7			1, 4
Rutile titanium dioxide	1317-80-2			8
Sand	308075-07-2			8

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Scandium oxide	12060-08-1			8
Sepiolite	63800-37-3			2
Silane, dichlorodimethyl-, reaction products with silica	68611-44-9			2, 4
<i>Silica</i>	7631-86-9			1, 2, 3, 4, 8
silica gel, cryst. -free	112926-00-8			3, 4
Silica, amorphous, fumed, cryst.-free	112945-52-5			1, 3, 4
Silica, vitreous	60676-86-0			1, 4, 8
Silicic acid, aluminum potassium sodium salt	12736-96-8			4
Siloxanes (Polysiloxane)	9011-19-2			4
Siloxanes and Silicones, di-Me, 3-hydroxypropyl Me, ethoxylated propoxylated	68937-55-3			8
Siloxanes and Silicones, di-Me, Me hydrogen	68037-59-2			8
Siloxanes and silicones, di-Me, polymers with Me silsesquioxanes	68037-74-1			4
Siloxanes and Silicones, di-Me, reaction products with silica	67762-90-7			4
Siloxanes and silicones, dimethyl,	63148-52-7			4
Silwet L77	27306-78-1			1
Sodium 1-octanesulfonate	5324-84-5	X		3
Sodium 2-mercaptobenzothiolate	2492-26-4	X		2
Sodium acetate	127-09-3	X		1, 3, 4
Sodium aluminate	1302-42-7			2, 4
Sodium benzoate	532-32-1	X		3
Sodium bicarbonate	144-55-8	X		1, 2, 3, 4, 7
Sodium bis(tridecyl) sulfobutanedioate	2673-22-5	X		4
Sodium bisulfite	7631-90-5			1, 3, 4
Sodium borate	1333-73-9			1, 4, 6, 7
Sodium bromate	7789-38-0			1, 2, 4
Sodium bromide	7647-15-6			1, 2, 3, 4, 7
Sodium bromosulfamate	1004542-84-0			8

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Sodium C14-16 alpha-olefin sulfonate	68439-57-6	X		1, 3, 4
Sodium caprylamphopropionate	68610-44-6	X		4
Sodium carbonate	497-19-8	X		1, 2, 3, 4, 8
Sodium chlorate	7775-09-9		X	1, 4
Sodium chloride	7647-14-5			1, 2, 3, 4, 5, 8
Sodium chlorite	7758-19-2		X	1, 2, 3, 4, 5, 8
Sodium chloroacetate	3926-62-3	X		3
Sodium cocaminopropionate	68608-68-4			1
Sodium decyl sulfate	142-87-0	X		1
Sodium D-gluconate	527-07-1	X		4
Sodium diacetate	126-96-5	X		1, 4
Sodium dichloroisocyanurate	2893-78-9	X		2
Sodium dl-lactate	72-17-3	X		8
Sodium dodecyl sulfate	151-21-3	X		8
Sodium erythorbate (1:1)	6381-77-7	X		1, 3, 4, 8
Sodium ethasulfate	126-92-1	X		1
Sodium formate	141-53-7	X		2, 8
Sodium hydrogen sulfate	7681-38-1			4
Sodium hydroxide	1310-73-2			1, 2, 3, 4, 7, 8
Sodium hydroxymethanesulfonate	870-72-4	X		8
Sodium hypochlorite	7681-52-9			1, 2, 3, 4, 8
Sodium iodide	7681-82-5		X	4
Sodium ligninsulfonate	8061-51-6			2
Sodium l-lactate	867-56-1	X		8
Sodium maleate (1:x)	18016-19-8	X		8
Sodium metabisulfite	7681-57-4			1
Sodium metaborate	7775-19-1			3, 4
Sodium metaborate dihydrate	16800-11-6			1, 4
Sodium metaborate tetrahydrate	10555-76-7			1, 4, 8
Sodium metasilicate	6834-92-0			1, 2, 4

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Sodium molybdate(VI)	7631-95-0			8
Sodium nitrate	7631-99-4			2
Sodium nitrite	7632-00-0			1, 2, 4
Sodium N-methyl-N-oleoyltaurate	137-20-2	X		4
Sodium octyl sulfate	142-31-4	X		1
Sodium oxide	1313-59-3			1
Sodium perborate	11138-47-9			4
Sodium perborate tetrahydrate	10486-00-7			1, 4, 5, 8
Sodium peroxoborate	7632-04-4			1
Sodium persulfate	7775-27-1			1, 2, 3, 4, 7, 8
Sodium phosphate	7632-05-5			1, 4
Sodium polyacrylate	9003-04-7			1, 2, 3, 4
Sodium pyrophosphate	7758-16-9		X	1, 2, 4
Sodium salicylate	54-21-7	X		1, 4
Sodium sesquicarbonate	533-96-0	X		1, 2
Sodium silicate	1344-09-8			1, 2, 4
Sodium starch glycolate	9063-38-1			2
Sodium sulfate	7757-82-6			1, 2, 3, 4
Sodium sulfite	7757-83-7			2, 4, 8
Sodium thiocyanate	540-72-7	X		1, 4
Sodium thiosulfate	7772-98-7			1, 2, 3, 4
Sodium thiosulfate, pentahydrate	10102-17-7			1, 4
Sodium trichloroacetate	650-51-1	X		1, 4
Sodium trimetaphosphate	7785-84-4		X	8
Sodium xylenesulfonate	1300-72-7	X		1, 3, 4
Sodium zirconium lactate	15529-67-6			8
Sodium zirconium lactic acid (4:4:1)	10377-98-7			1, 4
Solvent naphtha, petroleum, heavy aliph.	64742-96-7			2, 4, 8
Solvent naphtha, petroleum, heavy arom.	64742-94-5			1, 2, 4, 5, 8
Solvent naphtha, petroleum, light aliph.	64742-89-8			8

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Solvent naphtha, petroleum, light arom.	64742-95-6			1, 2, 4
Sorbic acid	110-44-1	X		8
Sorbitan sesquioleate	8007-43-0	X		4
Sorbitan, mono-(9Z)-9-octadecenoate	1338-43-8	X		1, 2, 3, 4
Sorbitan, monooctadecanoate	1338-41-6	X		8
Sorbitan, tri-(9Z)-9-octadecenoate	26266-58-0	X		8
Spirit of ammonia, aromatic	8013-59-0			8
Stannous chloride dihydrate	10025-69-1			1, 4
Starch	9005-25-8			1, 2, 4
Steam cracked distillate, cyclodiene dimer, dicyclopentadiene polymer	68131-87-3			1
Stoddard solvent	8052-41-3			1, 3, 4
Stoddard solvent IIC	64742-88-7			1, 2, 4
Strontium chloride	10476-85-4		X	4
Styrene	100-42-5	X	X	2
Subtilisin	9014-01-1			8
Sucrose	57-50-1	X		1, 2, 3, 4
Sulfamic acid	5329-14-6			1, 4
Sulfan blue	129-17-9	X		8
<i>Sulfate</i>	<i>14808-79-8</i>			<i>1, 4</i>
Sulfo NHS Biotin	119616-38-5			8
Sulfomethylated quebracho	68201-64-9			2
Sulfonic acids, C10-16-alkane, sodium salts	68608-21-9			6
Sulfonic acids, petroleum	61789-85-3			1
Sulfonic acids, petroleum, sodium salts	68608-26-4			3
Sulfur dioxide	7446-09-5			2, 4, 8
Sulfuric acid	7664-93-9			1, 2, 4, 7
Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	68955-19-1	X		4
Sulfuric acid, mono-C6-10-alkyl esters, ammonium salts	68187-17-7	X		1, 4, 8

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Symclosene	87-90-1	X		2
Talc	14807-96-6			1, 3, 4, 6, 7
Tall oil	8002-26-4			4, 8
Tall oil imidazoline	61791-36-4			4
Tall oil, compound with diethanolamine	68092-28-4			1
Tall oil, ethoxylated	65071-95-6			4, 8
Tall-oil pitch	8016-81-7			4
Tallow alkyl amines acetate	61790-60-1			8
Tar bases, quinoline derivatives, benzyl chloride-quaternized	72480-70-7			1, 3, 4
Tegin M	8043-29-6			8
Terpenes and Terpenoids, sweet orange-oil	68647-72-3			1, 3, 4, 8
Terpineol	8000-41-7			1, 3
tert-Butyl hydroperoxide	75-91-2	X		1, 4
tert-Butyl perbenzoate	614-45-9	X		1
Tetra-calcium-alumino-ferrite	12068-35-8			1, 2, 4
Tetradecane	629-59-4	X		8
Tetradecyldimethylbenzylammonium chloride	139-08-2	X		1, 4, 8
Tetraethylene glycol	112-60-7	X		1, 4
Tetraethylenepentamine	112-57-2	X		1, 4
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	X		1, 2, 3, 4, 7
Tetramethyl orthosilicate	681-84-5			1
Tetramethylammonium chloride	75-57-0	X		1, 2, 3, 4, 7, 8
Tetrasodium pyrophosphate	7722-88-5		X	8
Thiamine hydrochloride	67-03-8	X		8
Thiocyanic acid, ammonium salt	1762-95-4	X		2, 3, 4
Thioglycolic acid	68-11-1	X		1, 2, 3, 4
Thiourea	62-56-6	X	X	1, 2, 3, 4, 6
Thiourea, polymer with formaldehyde and 1-phenylethanone	68527-49-1			1, 4, 8
Thuja plicata donn ex. D. don leaf oil	68917-35-1			3

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Tin(II) chloride	7772-99-8			1
Titanium dioxide	13463-67-7			1, 2, 4
Titanium(4+) 2-[bis(2-hydroxyethyl)amino]ethanolate propan-2-olate (1:2:2)	36673-16-2			1
Titanium, isopropoxy (triethanolaminate)	74665-17-1			1, 4
<i>Toluene</i>	<i>108-88-3</i>	<b>X</b>	<b>X</b>	1, 3, 4
Tributyl phosphate	126-73-8	<b>X</b>	<b>X</b>	1, 2, 4
Tributyltetradecylphosphonium chloride	81741-28-8	<b>X</b>		1, 3, 4
Tricalcium phosphate	7758-87-4		<b>X</b>	1, 4
Tricalcium silicate	12168-85-3			1, 2, 4
Tridecane	629-50-5	<b>X</b>		8
Triethanolamine	102-71-6	<b>X</b>		1, 2, 4
Triethanolamine hydrochloride	637-39-8	<b>X</b>		8
Triethanolamine hydroxyacetate	68299-02-5	<b>X</b>		3
Triethanolamine polyphosphate ester	68131-71-5			1, 4, 8
Triethyl citrate	77-93-0	<b>X</b>		1, 4
Triethyl phosphate	78-40-0	<b>X</b>		1, 4
Triethylene glycol	112-27-6	<b>X</b>		1, 2, 3
Triethylenetetramine	112-24-3	<b>X</b>		4
Triisopropanolamine	122-20-3	<b>X</b>		1, 4
Trimethanolamine	14002-32-5	<b>X</b>		3
Trimethyl borate	121-43-7			8
Trimethylamine	75-50-3	<b>X</b>		8
Trimethylamine quaternized polyepichlorohydrin	51838-31-4			1, 2, 3, 4, 5, 8
Trimethylbenzene	25551-13-7			1, 2, 4
Triphosphoric acid, pentasodium salt	7758-29-4		<b>X</b>	1, 4
Tripoli	1317-95-9			4
Tripotassium citrate monohydrate	6100-05-6	<b>X</b>		4
Tripropylene glycol monomethyl ether	25498-49-1	<b>X</b>		2

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<b>Chemical name</b>	<b>CASRN</b>	<b>Physico-chemical properties</b>	<b>Selected toxicity reference value</b>	<b>Reference</b>
Trisodium citrate	68-04-2	X		3
Trisodium citrate dihydrate	6132-04-3	X		1, 4
Trisodium ethylenediaminetetraacetate	150-38-9	X		1, 3
Trisodium ethylenediaminetriacetate	19019-43-3	X		1, 4, 8
Trisodium phosphate	7601-54-9		X	1, 2, 4
Trisodium phosphate dodecahydrate	10101-89-0			1
Tritan R (X-100)	92046-34-9			8
Triton X-100	9002-93-1			1, 3, 4
Tromethamine	77-86-1	X		3, 4
Tryptone	73049-73-7			8
Ulexite	1319-33-1			1, 2, 3, 8
Undecane	1120-21-4	X		3, 8
Undecanol, branched and linear	128973-77-3			8
Urea	57-13-6	X		1, 2, 4, 8
Vermiculite	1318-00-9			2
Vinyl acetate ethylene copolymer	24937-78-8			1, 4
Vinylidene chloride/methylacrylate copolymer	25038-72-6			4
Water	7732-18-5			2, 4, 8
White mineral oil, petroleum	8042-47-5			1, 2, 4
<i>Xylenes</i>	1330-20-7	X	X	1, 2, 4
Yeast extract	8013-01-2			8
Zeolites	1318-02-1			8
<i>Zinc</i>	7440-66-6		X	2
Zinc carbonate	3486-35-9			2
Zinc chloride	7646-85-7			1, 2
Zinc oxide	1314-13-2			1, 4
Zinc sulfate monohydrate	7446-19-7			8
Zirconium nitrate	13746-89-9			2, 6
Zirconium oxide sulfate	62010-10-0			1, 4
Zirconium oxychloride	7699-43-6			1, 2, 4

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Zirconium(IV) chloride tetrahydrofuran complex	21959-01-3			5
Zirconium(IV) sulfate	14644-61-2			2, 6
Zirconium, 1,1'-((2-((2-hydroxyethyl)(2-hydroxypropyl)amino)ethyl)imino)bis(2-propanol) complexes	197980-53-3			4
Zirconium, acetate lactate oxo ammonium complexes	68909-34-2			4, 8
Zirconium, chloro hydroxy lactate oxo sodium complexes	174206-15-6			4
Zirconium, hydroxylactate sodium complexes	113184-20-6			1, 4
Zirconium,tetrakis[2-[bis(2-hydroxyethyl)amino-kN]ethanolato-kO]-	101033-44-7			1, 2, 4, 5

**Table A-3. List of generic names of chemicals reportedly used in hydraulic fracturing fluids.**

In some cases, the generic chemical name masks a specific chemical name and CASRN provided to the EPA and claimed as CBI by one or more of the nine hydraulic fracturing service companies.

Generic chemical name	Reference
2-Substituted aromatic amine salt	1, 4
Acetylenic alcohol	1
Acrylamide acrylate copolymer	4
Acrylamide copolymer	1, 4
Acrylamide modified polymer	4
Acrylamide-sodium acrylate copolymer	4
Acrylate copolymer	1
Acrylic copolymer	1
Acrylic polymer	1, 4
Acrylic resin	4
Acyclic hydrocarbon blend	1, 4
Acylbenzylpyridinium choride	8
Alcohol alkoxylate	1, 4
Alcohol and fatty acid blend	2

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<b>Generic chemical name</b>	<b>Reference</b>
Alcohol ethoxylates	4
Alcohols	1, 4
Alcohols, C9-C22	1, 4
Aldehydes	1, 4, 5
Alfa-alumina	1, 4
Aliphatic acids	1, 2, 3, 4
Aliphatic alcohol	2
Aliphatic alcohol glycol ether	3, 4
Aliphatic alcohols, ethoxylated	2
Aliphatic amine derivative	1
Aliphatic carboxylic acid	4
Alkaline bromide salts	1, 4
Alkaline metal oxide	4
Alkanes/alkenes	4
Alkanolamine derivative	2
Alkanolamine/aldehyde condensate	1, 2, 4
Alkenes	1, 4
Alklaryl sulfonic acid	1, 4
Alkoxyated alcohols	1
Alkoxyated amines	1, 4
Alkyaryl sulfonate	1, 2, 3, 4
Alkyl alkoxyate	1, 4
Alkyl amide	4
Alkyl amine	1, 4
Alkyl amine blend in a metal salt solution	1, 4
Alkyl aryl amine sulfonate	4
Alkyl aryl polyethoxy ethanol	3, 4
Alkyl dimethyl benzyl ammonium chloride	4
Alkyl esters	1, 4
Alkyl ether phosphate	4
Alkyl hexanol	1, 4
Alkyl ortho phosphate ester	1, 4

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<b>Generic chemical name</b>	<b>Reference</b>
Alkyl phosphate ester	1, 4
Alkyl phosphonate	4
Alkyl pyridines	2
Alkyl quaternary ammonium chlorides	1, 4
Alkyl quaternary ammonium salt	4
Alkylamine alkylaryl sulfonate	4
Alkylamine salts	2
Alkylaryl sulfonate	1, 4
Alkylated quaternary chloride	1, 2, 4
Alkylated sodium naphthalenesulphonate	2
Alkylbenzenesulfonate	2
Alkylbenzenesulfonic acid	1, 4, 5
Alkylethoammonium sulfates	1
Alkylphenol ethoxylates	1, 4
Alkylpyridinium quaternary	4
Aliphatic alcohol polyglycol ether	2
Aluminum oxide	1, 4
Amide	4
Amidoamine	1, 4
Amine	1, 4
Amine compound	4
Amine oxides	1, 4
Amine phosphonate	1, 4
Amine salt	1
Amino compounds	1, 4
Amino methylene phosphonic acid salt	1, 4
Ammonium alcohol ether sulfate	1, 4
Ammonium salt	1, 4
Ammonium salt of ethoxylated alcohol sulfate	1, 4
Amorphous silica	4
Amphoteric surfactant	2
Anionic acrylic polymer	2

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<b>Generic chemical name</b>	<b>Reference</b>
Anionic copolymer	1, 4
Anionic polyacrylamide	1, 2, 4
Anionic polyacrylamide copolymer	1, 4, 6
Anionic polymer	1, 3, 4
Anionic surfactants	2, 4, 6
Antifoulant	1, 4
Antimonate salt	1, 4
Aqueous emulsion of diethylpolysiloxane	2
Aromatic alcohol glycol ether	1
Aromatic aldehyde	1, 4
Aromatic hydrocarbons	3, 4
Aromatic ketones	1, 2, 3, 4
Aromatic polyglycol ether	1
Arsenic compounds	4
Ashes, residues	4
Bentone clay	4
Biocide	4
Biocide component	1, 4
Bis-quaternary methacrylamide monomer	4
Blast furnace slag	4
Borate salts	1, 2, 4
Cadmium compounds	4
Carbohydrates	1, 2, 4
Carboxymethyl hydroxypropyl guar	4
Cationic polyacrylamide	4
Cationic polymer	2, 4
Cedar fiber, processed	2
Cellulase enzyme	1
Cellulose derivative	1, 2, 4
Cellulose ether	2
Cellulosic polymer	2
Ceramic	4

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<b>Generic chemical name</b>	<b>Reference</b>
Chlorous ion solution	1
Chromates	1, 4
Chrome-free lignosulfonate compound	2
Citrus rutaceae extract	4
Common white	4
Complex alkylaryl polyo-ester	1
Complex aluminum salt	1, 4
Complex carbohydrate	2
Complex organometallic salt	1
Complex polyamine salt	7
Complex substituted keto-amine	1
Complex substituted keto-amine hydrochloride	1
Copper compounds	6
Coric oxide	4
Cotton dust (raw)	2
Cottonseed hulls	2
Cured acrylic resin	1, 4
Cured resin	1, 4, 5
Cured urethane resin	1, 4
Cyclic alkanes	1, 4
Defoamer	4
Dibasic ester	4
Dicarboxylic acid	1, 4
Diesel	1, 4, 6
Dimethyl silicone	1, 4
Dispersing agent	1
Emulsifier	4
Enzyme	4
Epoxy	4
Epoxy resin	1, 4
Essential oils	1, 4
Ester Salt	2, 4

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<b>Generic chemical name</b>	<b>Reference</b>
Esters	2, 4
Ether compound	4
Ether salt	4
Ethoxylated alcohol blend	4
Ethoxylated alcohol/ester mixture	4
Ethoxylated alcohols	1, 2, 4, 5, 7
Ethoxylated alkyl amines	1, 4
Ethoxylated amine blend	4
Ethoxylated amines	1, 4
Ethoxylated fatty acid	4
Ethoxylated fatty acid ester	1, 4
Ethoxylated nonionic surfactant	1, 4
Ethoxylated nonylphenol	1, 2, 4
Ethoxylated sorbitol esters	1, 4
Ethylene oxide-nonylphenol polymer	4
Fatty acid amine salt mixture	4
Fatty acid ester	1, 2, 4
Fatty acid tall oil	1, 4
Fatty acid, ethoxylate	4
Fatty acids	1
Fatty alcohol alkoxyate	1, 4
Fatty alkyl amine salt	1, 4
Fatty amine carboxylates	1, 4
Fatty imidazoline	4
Fluoroaliphatic polymeric esters	1, 4
Formaldehyde polymer	1
Glass fiber	1, 4
Glyceride esters	2
Glycol	4
Glycol blend	2
Glycol ethers	1, 4, 7
Ground cedar	2

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<b>Generic chemical name</b>	<b>Reference</b>
Ground paper	2
Guar derivative	1, 4
Guar gum	4
Haloalkyl heteropolycycle salt	1, 4
Hexanes	1
High molecular weight polymer	2
High pH conventional enzymes	2
Hydrocarbons	1
Hydrogen solvent	4
Hydrotreated and hydrocracked base oil	1, 4
Hydrotreated distillate, light C9-16	4
Hydrotreated heavy naphthalene	5
Hydrotreated light distillate	2, 4
Hydrotreated light petroleum distillate	4
Hydroxyalkyl imino carboxylic sodium salt	2
Hydroxycellulose	6
Hydroxyethyl cellulose	1, 2, 4
Imidazolium compound	4
Inner salt of alkyl amines	1, 4
Inorganic borate	1, 4
Inorganic chemical	4
Inorganic particulate	1, 4
Inorganic salt	2, 4
Iso-alkanes/n-alkanes	1, 4
Isomeric aromatic ammonium salt	1, 4
Latex	2, 4
Lead compounds	4
Low toxicity base oils	1, 4
Lubra-Beads course	4
Maghemite	1, 4
Magnetite	1, 4
Metal salt	1

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<b>Generic chemical name</b>	<b>Reference</b>
Metal salt solution	1
Mineral	1, 4
Mineral fiber	2
Mineral filler	1
Mineral oil	4
Mixed titanium ortho ester complexes	1, 4
Modified acrylamide copolymer	2, 4
Modified acrylate polymer	4
Modified alkane	1, 4
Modified bentonite	4
Modified cycloaliphatic amine adduct	1, 4
Modified lignosulfonate	2, 4
Naphthalene derivatives	1, 4
Neutralized alkylated naphthalene sulfonate	4
Nickel chelate catalyst	4
Nonionic surfactant	1
N-tallowalkyltrimethylenediamines	4
Nuisance particulates	1, 2, 4
Nylon	4
Olefinic sulfonate	1, 4
Olefins	1, 4
Organic acid salt	1, 4
Organic acids	1, 4
Organic alkyl amines	4
Organic chloride	4
Organic modified bentonite clay	4
Organic phosphonate	1, 4
Organic phosphonate salts	1, 4
Organic phosphonic acid salts	1, 4
Organic polymer	4
Organic polyol	4
Organic salt	1, 4

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<b>Generic chemical name</b>	<b>Reference</b>
Organic sulfur compound	1, 4
Organic surfactants	1
Organic titanate	1, 4
Organo amino silane	4
Organo phosphonic acid	4
Organo phosphonic acid salt	4
Organometallic ammonium complex	1
Organophilic clay	4
Oxidized tall oil	2
Oxoaliphatic acid	2
Oxyalkylated alcohol	1, 4
Oxyalkylated alkyl alcohol	2, 4
Oxyalkylated alkylphenol	1, 2, 3, 4
Oxyalkylated fatty acid	1, 4
Oxyalkylated fatty alcohol salt	2
Oxyalkylated phenol	1, 4
Oxyalkylated phenolic resin	4
Oxyalkylated polyamine	1
Oxyalkylated tallow diamine	2
Oxyethylated alcohol	2
Oxylated alcohol	1, 4
P/F resin	4
Paraffin inhibitor	4
Paraffinic naphthenic solvent	1
Paraffinic solvent	1, 4
Paraffins	1
Pecan shell	2
Petroleum distillate blend	2, 3, 4
Petroleum gas oils	1
Petroleum hydrocarbons	4
Petroleum solvent	2
Phosphate ester	1, 4

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<b>Generic chemical name</b>	<b>Reference</b>
Phosphonate	2
Phosphonic acid	1, 4
Phosphoric acid, mixed polyoxyalkylene aryl and alkyl esters	4
Plasticizer	1, 2
Polyacrylamide copolymer	4
Polyacrylamides	1
Polyacrylate	1, 4
Polyactide resin	4
Polyalkylene esters	4
Polyaminated fatty acid	2
Polyaminated fatty acid surfactants	2
Polyamine	1, 4
Polyamine polymer	4
Polyanionic cellulose	1
Polyaromatic hydrocarbons	6
Polycyclic organic matter	6
Polyelectrolyte	4
Polyether polyol	2
Polyethoxylated alkanol	2, 3, 4
Polyethylene copolymer	4
Polyethylene glycols	4
Polyethylene wax	4
Polyglycerols	2
Polyglycol	2
Polyglycol ether	6
Poly lactide resin	4
Polymer	2, 4
Polymeric hydrocarbons	3, 4
Polymerized alcohol	4
Polymethacrylate polymer	4
Polyol phosphate ester	2
Polyoxyalkylene phosphate	2

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<b>Generic chemical name</b>	<b>Reference</b>
Polyoxyalkylene sulfate	2
Polyoxyalkylenes	1, 4, 7
Polyphenylene ether	4
Polyphosphate	4
Polypropylene glycols	2
Polyquaternary amine	4
Polysaccharide polymers in suspension	2
Polysaccharide	4
Polysaccharide blend	4
Polyvinylalcohol/polyvinylacetate copolymer	4
Potassium chloride substitute	4
Quaternized heterocyclic amines	4
Quaternary amine	2, 4
Quaternary amine salt	4
Quaternary ammonium chloride	4
Quaternary ammonium compound	1, 2, 4
Quaternary ammonium salts	1, 2, 4
Quaternary compound	1, 4
Quaternary salt	1, 4
Quaternized alkyl nitrogenated compd	4
Red dye	4
Refined mineral oil	2
Resin	4
Salt of amine-carbonyl condensate	3, 4
Salt of fatty acid/polyamine reaction product	3, 4
Salt of phosphate ester	1
Salt of phosphono-methylated diamine	1, 4
Salts	4
Salts of oxyalkylated fatty amines	4
Sand	4
Sand, AZ silica	4
Sand, brown	4

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<b>Generic chemical name</b>	<b>Reference</b>
Sand, sacked	4
Sand, white	4
Secondary alcohol	1, 4
Silica sand, 100 mesh, sacked	4
Silicone emulsion	1
Silicone ester	4
Sodium acid pyrophosphate	4
Sodium calcium magnesium polyphosphate	4
Sodium phosphate	4
Sodium salt of aliphatic amine acid	2
Sodium xylene sulfonate	4
Softwood dust	2
Starch blends	6
Substituted alcohol	1, 2, 4
Substituted alkene	1
Substituted alkylamine	1, 4
Substituted alkyne	4
Sulfate	4
Sulfomethylated tannin	2, 5
Sulfonate	4
Sulfonate acids	1
Sulfonate surfactants	1
Sulfonated asphalt	2
Sulfonic acid salts	1, 4
Sulfur compound	1, 4
Sulphonic amphoteric	4
Sulphonic amphoteric blend	4
Surfactant blend	3, 4
Surfactants	1, 2, 4
Synthetic copolymer	2
Synthetic polymer	4
Tallow soap	4

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Generic chemical name	Reference
Telomer	4
Terpenes	1, 4
Titanium complex	4
Triethanolamine zirconium chelate	1 4
Triterpanes	4
Vanadium compounds	4
Wall material	1
Walnut hulls	1, 2, 4
Zirconium complex	2, 4
Zirconium salt	4

**Table A-4. Chemicals detected in flowback or produced water.**

An “X” indicates the availability of physicochemical properties from EPI Suite™ and selected toxicity reference values (see Appendix G). An empty cell indicates no information was available from the sources we consulted. Reference number corresponds to the citations in Table A-1. Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
1,2,3-Trichlorobenzene	87-61-6	X	X	3, 9
1,2,4-Trichlorobenzene	120-82-1	X	X	9
<i>1,2,4-Trimethylbenzene</i>	<i>95-63-6</i>	X		<i>3, 9, 10</i>
<i>1,2-Propylene glycol</i>	<i>57-55-6</i>	X	X	<i>3, 9</i>
<i>1,3,5-Trimethylbenzene</i>	<i>108-67-8</i>	X		<i>3, 9, 10</i>
<i>1,4-Dioxane</i>	<i>123-91-1</i>	X	X	<i>9, 10</i>
2,4-Dimethylphenol	105-67-9	X	X	3, 9, 10
2,6-Dichlorophenol	87-65-0	X		3, 9
2-Methylnaphthalene	91-57-6	X	X	3, 9, 10
2-Methylpropanoic acid	79-31-2	X		10
2-Methylpyridine	109-06-8	X		3, 9
7,12-Dimethylbenz(a)anthracene	57-97-6	X	X	3, 9
<i>Acetic acid</i>	<i>64-19-7</i>	X		<i>3, 9, 10</i>

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<b>Chemical name</b>	<b>CASRN</b>	<b>Physico-chemical properties</b>	<b>Selected toxicity reference value</b>	<b>Reference</b>
<i>Acetone</i>	67-64-1	X	X	3, 9, 10
<i>Acetophenone</i>	98-86-2	X	X	3, 9
<i>Acrolein</i>	107-02-8	X	X	9
Acrylonitrile	107-13-1	X	X	3, 9
Aldrin	309-00-2	X	X	3, 9
<i>Aluminum</i>	7429-90-5		X	3, 9, 10
<i>Ammonia</i>	7664-41-7			3, 9, 10
Antimony	7440-36-0		X	3, 9, 10
Aroclor 1248	12672-29-6	X		3, 9
<i>Arsenic</i>	7440-38-2		X	3, 9, 10
Barium	7440-39-3		X	3, 9, 10
<i>Benzene</i>	71-43-2	X	X	3, 9, 10
Benzo(a)pyrene	50-32-8	X	X	3, 9
Benzo(b)fluoranthene	205-99-2	X	X	3, 9
Benzo(g,h,i)perylene	191-24-2	X		3, 9, 10
Benzo(k)fluoranthene	207-08-9	X	X	3, 9
Benzyl alcohol	100-51-6	X	X	3, 9, 10
Beryllium	7440-41-7		X	3, 9, 10
beta-Hexachlorocyclohexane	319-85-7	X	X	3, 9
<i>Bis(2-chloroethyl) ether</i>	111-44-4	X	X	3, 9
Boron	7440-42-8		X	3, 9, 10
Bromide	24959-67-9			3, 9, 10
Bromodichloromethane	75-27-4	X	X	3
Bromoform	75-25-2	X	X	3, 9, 10
Butanoic acid	107-92-6	X		9, 10
Butylbenzene	104-51-8	X	X	9, 10
Cadmium	7440-43-9		X	3, 9, 10
Caesium-137	10045-97-3			3
Calcium	7440-70-2			3, 9, 10
<i>Carbon dioxide</i>	124-38-9	X		3, 9, 10

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<b>Chemical name</b>	<b>CASRN</b>	<b>Physico-chemical properties</b>	<b>Selected toxicity reference value</b>	<b>Reference</b>
Carbon disulfide	75-15-0	X	X	3, 9
<i>Chloride</i>	16887-00-6			3, 9, 10
<i>Chlorine</i>	7782-50-5		X	3, 10
Chlorodibromomethane	124-48-1	X	X	3
Chloroform	67-66-3	X	X	3, 9, 10
Chloromethane	74-87-3	X		3, 10
Chromium	7440-47-3			3, 9, 10
<i>Chromium (III)</i>	16065-83-1		X	3
<i>Chromium (VI)</i>	18540-29-9		X	3, 10
Cobalt	7440-48-4		X	3, 9, 10
<i>Copper</i>	7440-50-8		X	3, 9, 10
<i>Cumene</i>	98-82-8	X	X	3, 9
Cyanide	57-12-5	X	X	3, 9, 10
delta-Hexachlorocyclohexane	319-86-8	X		9
<i>Di(2-ethylhexyl) phthalate</i>	117-81-7	X	X	3, 9, 10
Dibenz(a,h)anthracene	53-70-3	X	X	3, 9
Dibutyl phthalate	84-74-2	X	X	3, 9, 10
<i>Dichloromethane</i>	75-09-2	X	X	9, 10
Dieldrin	60-57-1	X	X	9
Diethyl phthalate	84-66-2	X	X	9
Diocetyl phthalate	117-84-0	X	X	9, 10
Diphenylamine	122-39-4	X	X	3, 9
Endosulfan I	959-98-8	X		3, 9
Endosulfan II	33213-65-9	X		3, 9
Endrin aldehyde	7421-93-4	X		3, 9
<i>Ethylbenzene</i>	100-41-4	X	X	3, 9, 10
<i>Ethylene glycol</i>	107-21-1	X	X	3, 9
Fluoranthene	206-44-0	X	X	3, 9
Fluorene	86-73-7	X	X	3, 9, 10
Fluoride	16984-48-8			3, 9, 10

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<b>Chemical name</b>	<b>CASRN</b>	<b>Physico-chemical properties</b>	<b>Selected toxicity reference value</b>	<b>Reference</b>
<i>Formic acid</i>	64-18-6	X	X	10
Heptachlor	76-44-8	X	X	3, 9
Heptachlor epoxide	1024-57-3	X	X	3, 9
Heptanoic acid	111-14-8	X		10
Hexanoic acid	142-62-1	X		10
Indeno(1,2,3-cd)pyrene	193-39-5	X	X	3, 9
<i>Iron</i>	7439-89-6		X	3, 9, 10
<i>Isopropanol</i>	67-63-0	X		3, 9
Isovaleric acid	503-74-2	X		10
<i>Lead</i>	7439-92-1		X	3, 9, 10
Lindane	58-89-9	X	X	3, 9
Lithium	7439-93-2		X	3, 9, 10
Magnesium	7439-95-4			3, 9, 10
Manganese	7439-96-5		X	3, 9, 10
m-Cresol	108-39-4	X	X	3, 9, 10
Mercury	7439-97-6		X	3, 9, 10
<i>Methanol</i>	67-56-1	X	X	3, 9
Methyl bromide	74-83-9	X	X	3, 9
Methyl ethyl ketone	78-93-3	X	X	3, 9, 10
Molybdenum	7439-98-7		X	3, 9, 10
<i>Naphthalene</i>	91-20-3	X	X	3, 9, 10
Nickel	7440-02-0			3, 9, 10
Nitrate	14797-55-8		X	3, 9, 10
Nitrite	14797-65-0		X	3, 9, 10
N-Nitrosodiphenylamine	86-30-6	X	X	3, 9
o-Cresol	95-48-7	X	X	3, 9, 10
p,p'-DDE	72-55-9	X	X	3, 9
p-Cresol	106-44-5	X	X	3, 9, 10
p-Cymene	99-87-6	X		9, 10
Pentanoic acid	109-52-4	X		10

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<b>Chemical name</b>	<b>CASRN</b>	<b>Physico-chemical properties</b>	<b>Selected toxicity reference value</b>	<b>Reference</b>
<i>Phenanthrene</i>	85-01-8	X		3, 9, 10
<i>Phenol</i>	108-95-2	X	X	3, 9, 10
Phorate	298-02-2	X	X	9
Phosphorus	7723-14-0		X	3, 9
Potassium	7440-09-7			3, 9, 10
Propionic acid	79-09-4	X		10
Propylbenzene	103-65-1	X		9
Pyrene	129-00-0	X	X	9, 10
Pyridine	110-86-1	X	X	3, 9, 10
Radium	7440-14-4			3
Radium-226	13982-63-3			3, 10
Radium-228	15262-20-1			3, 10
Safrole	94-59-7	X	X	3, 9
sec-Butylbenzene	135-98-8	X		9
Selenium	7782-49-2		X	3, 9, 10
<i>Silica</i>	7631-86-9			10
Silicon	7440-21-3			10
Silver	7440-22-4		X	3, 9, 10
Sodium	7440-23-5			3, 9, 10
Strontium	7440-24-6		X	3, 9, 10
<i>Sulfate</i>	14808-79-8			3, 9, 10
Sulfite	14265-45-3			3
Tetrachloroethylene	127-18-4	X	X	3, 9
Thallium	7440-28-0			3, 9, 10
Tin	7440-31-5		X	9, 10
Titanium	7440-32-6			3, 9, 10
<i>Toluene</i>	108-88-3	X	X	3, 9, 10
Vanadium	7440-62-2		X	3, 10

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Chemical name	CASRN	Physico-chemical properties	Selected toxicity reference value	Reference
Xylenes	1330-20-7	X	X	3, 9, 10
Zinc	7440-66-6		X	3, 9, 10
Zirconium	7440-67-7			3

## A.2. References for Appendix A

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## Appendix B

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### Water Acquisition Tables

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## Appendix B. Water Acquisition Tables

### B.1. Supplemental Tables

**Table B-1. Annual average hydraulic fracturing water use and consumption in 2011 and 2012 compared to total annual water use and consumption in 2010 by state.**

Hydraulic fracturing water use data from the EPA's project database of disclosures to FracFocus 1.0 ([U.S. EPA, 2015c](#)). Annual total water use data from the U.S. Geological Survey (USGS) Water Census ([Maupin et al., 2014](#)). Estimates of consumptions derived from hydraulic fracturing water use and total water use data. States listed in descending order by the volume of hydraulic fracturing water use.

State	Total annual water use in 2010 (millions of gal) <sup>a,b</sup>	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal) <sup>c</sup>	Hydraulic fracturing water use compared to total water use (%) <sup>d</sup>	Hydraulic fracturing water consumption compared to total water consumption (%) <sup>d,e</sup>
Texas	9,052,000	19,942	0.2	0.7
Pennsylvania	2,967,450	5,105	0.2	1.4
Arkansas	4,124,500	3,676	0.1	0.1
Colorado	4,015,000	3,277	0.1	0.1
Oklahoma	1,157,050	2,949	0.3	0.8
Louisiana	3,117,100	2,462	0.1	0.4
North Dakota	419,750	2,181	0.5	2.9
West Virginia	1,288,450	657	0.1	0.5
Wyoming	1,715,500	538	<0.1	<0.1
New Mexico	1,153,400	371	<0.1	<0.1
Ohio	3,445,600	273	<0.1	0.1
Utah	1,627,900	251	<0.1	<0.1
Montana	2,792,250	155	<0.1	<0.1
Kansas	1,460,000	66	<0.1	<0.1
California	13,870,000	44	<0.1	<0.1
Michigan	3,942,000	28	<0.1	<0.1

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State	Total annual water use in 2010 (millions of gal) <sup>a,b</sup>	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal) <sup>c</sup>	Hydraulic fracturing water use compared to total water use (%) <sup>d</sup>	Hydraulic fracturing water consumption compared to total water consumption (%) <sup>d,e</sup>
Mississippi	1,434,450	18	<0.1	<0.1
Alaska <sup>f</sup>	397,850	7	<0.1	<0.1
Virginia	2,792,250	1	<0.1	<0.1
Alabama	3,635,400	1	<0.1	<0.1
TOTAL for all 20 states	64,407,900	42,001	0.1	0.2

<sup>a</sup> Texas, Colorado, Pennsylvania, North Dakota, Oklahoma, and Utah all made some degree of reporting to FracFocus mandatory rather than voluntary during this time period analyzed, January 1, 2011, to February 28, 2013. Three other states started requiring disclosure to either FracFocus or the state (Louisiana, Montana, and Ohio), and five states required or began requiring disclosure to the state (Arkansas, Michigan, New Mexico, West Virginia, and Wyoming). Alabama, Alaska, California, Kansas, Mississippi, and Virginia did not have reporting requirements during the period of time studied ([U.S. EPA, 2015a](#)).

<sup>b</sup> State-level data accessed from the USGS website (<http://water.usgs.gov/watuse/data/2010/>) on January 27, 2015. Total water withdrawals per day (located in downloaded Table 1) were multiplied by 365 days to estimate total water use for the year ([Maupin et al., 2014](#)).

<sup>c</sup> Average of water used for hydraulic fracturing in 2011 and 2012 as reported to FracFocus ([U.S. EPA, 2015c](#)).

<sup>d</sup> Percentages were calculated by averaging annual water use for hydraulic fracturing reported in FracFocus in 2011 and 2012 for a given state ([U.S. EPA, 2015c](#)), and then dividing by 2010 USGS hydraulic fracturing water use ([Maupin et al., 2014](#)) and multiplying by 100. Note that the annual hydraulic fracturing water use reported in FracFocus (the numerator) was not added to the 2010 total USGS water use value in the denominator, and the percentage is simply calculated as by dividing annual hydraulic fracturing use by 2010 total water use or consumption. This was done because of the difference in years between the two datasets, and because the USGS 2010 Census ([Maupin et al., 2014](#)) already included an estimate of hydraulic fracturing water use in its mining category. This approach is also consistent with that of other literature on this topic; see [Nicot and Scanlon \(2012\)](#).

<sup>e</sup> Consumption values were calculated with use-specific consumption rates predominantly from the USGS, including 19.2% for public supply, 19.2% for domestic use, 60.7% for irrigation, 60.7% for livestock, 14.8% for industrial uses, 14.8% for mining ([Solley et al., 1998](#)), and 2.7% for thermoelectric power ([USGS, 2014](#)). We used a rate of 71.6% for aquaculture ([from Verdegem and Bosma, 2009](#)) (evaporation per kg fish + infiltration per kg)/(total water use per kg) \*100. These rates were multiplied by each USGS water use value ([Maupin et al., 2014](#)) to yield a total water consumption estimate. To calculate a consumption amount for hydraulic fracturing, we used a consumption rate of 82.5%. This was calculated by taking the median value for all reported produced water/injected water percentages in Tables 7-1 and 7-2 of this assessment and then subtracting from 100%. If a range of values was given, the midpoint was used. Note that this is likely a low estimate of consumption since much of this return water is not subsequently treated and reused, but rather disposed of in underground injection wells—see Chapter 8.

<sup>f</sup> All reported hydraulic fracturing disclosures for Alaska passed state locational quality assurance methods, but not county methods ([U.S. EPA, 2015c](#)). Thus, only state-level cumulative values were reported here, and no county-level data are provided in subsequent tables.

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**Table B-2. Annual average hydraulic fracturing water use and consumption in 2011 and 2012 compared to total annual water use and consumption in 2010 by county.**

Counties listed contained wells used for hydraulic fracturing according to the EPA's project database of disclosures to FracFocus 1.0 ([U.S. EPA, 2015c](#)). Annual total water use data from the USGS Water Census ([Maupin et al., 2014](#)). Estimates of consumption derived from hydraulic fracturing water use and total water use data.

State	County	Total annual water use in 2010 (millions of gal) <sup>a</sup>	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal) <sup>b</sup>	Hydraulic fracturing water use compared to total water use (%) <sup>c</sup>	Hydraulic fracturing water consumption compared to total water consumption (%) <sup>c,d</sup>
Alabama	Jefferson	29,685.5	0.6	<0.1	<0.1
	Tuscaloosa	14,319.0	0.5	<0.1	<0.1
Arkansas	Cleburne	9,471.8	740.9	7.8	32.9
	Conway	10,643.4	798.1	7.5	21.2
	Faulkner	3,204.7	284.0	8.9	13.7
	Independence	57,195.5	80.3	0.1	0.3
	Logan	1,525.7	2.4	0.2	0.3
	Sebastian	1,365.1	0.6	<0.1	<0.1
	Van Buren	1,587.8	899.6	56.7	168.8
	White	32,131.0	869.8	2.7	4.7
	Yell	1,507.5	<0.1	<0.1	<0.1
California	Colusa	304,782.3	<0.1	<0.1	<0.1
	Glenn	221,420.0	<0.1	<0.1	<0.1
	Kern	788,359.9	41.7	<0.1	<0.1
	Los Angeles	1,118,363.7	0.2	<0.1	<0.1
	Sutter	263,511.8	0.2	<0.1	<0.1
	Ventura	262,610.2	1.8	<0.1	<0.1
Colorado	Adams	84,285.8	3.2	<0.1	<0.1
	Arapahoe	68,255.0	4.0	<0.1	<0.1
	Boulder	84,537.7	4.1	<0.1	<0.1

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State	County	Total annual water use in 2010 (millions of gal) <sup>a</sup>	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal) <sup>b</sup>	Hydraulic fracturing water use compared to total water use (%) <sup>c</sup>	Hydraulic fracturing water consumption compared to total water consumption (%) <sup>c,d</sup>
Colorado, cont.	Broomfield	2,336.0	4.5	0.2	0.4
	Delta	131,221.2	0.5	<0.1	<0.1
	Dolores	2,040.4	0.1	<0.1	<0.1
	El Paso	42,380.2	<0.1	<0.1	<0.1
	Elbert	5,040.7	<0.1	<0.1	<0.1
	Fremont	53,366.7	0.6	<0.1	<0.1
	Garfield	95,436.6	1,804.2	1.9	2.7
	Jackson	126,968.9	1.0	<0.1	<0.1
	La Plata	122,873.6	3.5	<0.1	<0.1
	Larimer	150,690.3	5.4	<0.1	<0.1
	Las Animas	26,911.5	7.9	<0.1	<0.1
	Mesa	275,476.5	122.1	<0.1	0.1
	Moffat	62,093.8	14.5	<0.1	<0.1
	Morgan	67,901.0	3.9	<0.1	<0.1
	Phillips	21,509.5	0.2	<0.1	<0.1
	Rio Blanco	97,513.4	147.3	0.2	0.2
	Routt	74,460.0	0.1	<0.1	<0.1
	San Miguel	13,848.1	0.3	<0.1	<0.1
	Weld	168,677.5	1,149.4	0.7	1.0
	Yuma	80,595.7	0.4	<0.1	<0.1
Kansas	Barber	2,164.5	9.9	0.5	0.7
	Clark	1,898.0	0.8	<0.1	0.1
	Comanche	3,011.3	25.6	0.9	1.2
	Finney	102,685.5	2.4	<0.1	<0.1
	Grant	47,128.8	0.2	<0.1	<0.1

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State	County	Total annual water use in 2010 (millions of gal) <sup>a</sup>	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal) <sup>b</sup>	Hydraulic fracturing water use compared to total water use (%) <sup>c</sup>	Hydraulic fracturing water consumption compared to total water consumption (%) <sup>c,d</sup>
Kansas, cont.	Gray	69,379.2	3.3	<0.1	<0.1
	Harper	1,357.8	17.3	1.3	2.0
	Haskell	72,496.3	0.1	<0.1	<0.1
	Hodgeman	8,460.7	2.7	<0.1	<0.1
	Kearny	64,134.2	<0.1	<0.1	<0.1
	Lane	5,628.3	0.8	<0.1	<0.1
	Meade	55,958.2	<0.1	<0.1	<0.1
	Morton	17,403.2	<0.1	<0.1	<0.1
	Ness	1,478.3	1.6	0.1	0.2
	Seward	57,443.7	<0.1	<0.1	<0.1
	Sheridan	26,393.2	0.7	<0.1	<0.1
	Stanton	41,420.2	<0.1	<0.1	<0.1
	Stevens	72,124.0	0.1	<0.1	<0.1
	Sumner	3,442.0	0.2	<0.1	<0.1
Louisiana	Allen	8,942.5	0.1	<0.1	<0.1
	Beauregard	10,161.6	2.3	<0.1	0.1
	Bienville	4,810.7	108.9	2.3	10.0
	Bossier	5,599.1	110.1	2.0	4.9
	Caddo	53,644.1	153.6	0.3	1.7
	Calcasieu	81,621.3	0.1	<0.1	<0.1
	Caldwell	1,398.0	<0.1	<0.1	<0.1
	Claiborne	952.7	3.8	0.4	1.1
	De Soto	13,373.6	1,085.9	8.1	47.4
	East Feliciana	1,350.5	3.7	0.3	0.7
	Jackson	1,456.4	<0.1	<0.1	<0.1

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State	County	Total annual water use in 2010 (millions of gal) <sup>a</sup>	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal) <sup>b</sup>	Hydraulic fracturing water use compared to total water use (%) <sup>c</sup>	Hydraulic fracturing water consumption compared to total water consumption (%) <sup>c,d</sup>
Louisiana, cont.	Lincoln	3,000.3	3.3	0.1	0.3
	Natchitoches	12,530.5	12.7	0.1	0.2
	Rapides	199,976.2	1.7	<0.1	<0.1
	Red River	1,606.0	569.6	35.5	83.2
	Sabine	1,522.1	395.2	26.0	76.6
	Tangipahoa	7,329.2	1.9	<0.1	0.1
	Union	1,481.9	4.9	0.3	1.0
	Webster	2,664.5	1.2	<0.1	0.1
	West Feliciana	15,191.3	2.3	<0.1	0.1
	Winn	846.8	1.1	0.1	0.4
Michigan	Cheboygan	2,777.7	<0.1	<0.1	<0.1
	Gladwin	850.5	1.1	0.1	0.4
	Kalkaska	1,233.7	24.0	1.9	3.7
	Missaukee	1,423.5	<0.1	<0.1	<0.1
	Ogemaw	1,179.0	<0.1	<0.1	<0.1
	Roscommon	1,000.1	2.4	0.2	0.9
Mississippi	Amite	792.1	14.4	1.8	3.8
	Wilkinson	1,270.2	3.2	0.3	0.4
Montana	Daniels	1,408.9	0.6	<0.1	0.1
	Garfield	1,631.6	0.5	<0.1	<0.1
	Glacier	46,760.2	5.1	<0.1	<0.1
	Musselshell	26,827.5	0.4	<0.1	<0.1
	Richland	94,797.8	83.5	0.1	0.1

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Montana, cont.	Roosevelt	31,539.7	52.1	0.2	0.2
	Rosebud	71,412.3	3.5	<0.1	<0.1
	Sheridan	7,354.8	9.7	0.1	0.2
New Mexico	Chaves	88,078.2	2.8	<0.1	<0.1
	Colfax	17,450.7	0.7	<0.1	<0.1
	Eddy	70,612.9	225.6	0.3	0.5
	Harding	1,168.0	0.1	<0.1	<0.1
	Lea	64,057.5	113.7	0.2	0.3
	Rio Arriba	39,080.6	16.5	<0.1	0.1
	Roosevelt	63,367.7	<0.1	<0.1	<0.1
	San Juan	125,432.3	11.6	<0.1	<0.1
	Sandoval	23,922.1	0.4	<0.1	<0.1
North Dakota	Billings	762.9	44.4	5.8	16.2
	Bottineau	1,164.4	0.1	<0.1	<0.1
	Burke	394.2	63.6	16.1	40.8
	Divide	806.7	102.2	12.7	18.6
	Dunn	1,076.8	309.5	28.7	43.1
	Golden Valley	208.1	4.6	2.2	3.8
	Mckenzie	13,753.2	588.4	4.3	6.2
	Mclean	7,873.1	12.2	0.2	0.4
	Mountrail	1,248.3	449.4	36.0	98.3
	Stark	1,168.0	48.0	4.1	8.5
	Williams	7,705.2	558.5	7.2	11.3

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Ohio	Ashland	2,033.1	1.5	0.1	0.2
	Belmont	65,528.5	1.9	<0.1	0.1
	Carroll	1,127.9	152.7	13.5	37.3
	Columbiana	3,763.2	30.7	0.8	2.2
	Coshocton	53,775.5	5.4	<0.1	0.1
	Guernsey	2,379.8	8.4	0.4	0.7
	Harrison	481.8	16.5	3.4	7.3
	Jefferson	632,917.3	26.2	<0.1	0.1
	Knox	3,270.4	1.1	<0.1	0.1
	Medina	3,540.5	1.3	<0.1	0.1
	Muskingum	6,018.9	5.1	0.1	0.3
	Noble	478.2	8.3	1.7	3.4
	Portage	18,414.3	3.2	<0.1	0.1
	Stark	16,479.8	2.4	<0.1	<0.1
	Tuscarawas	14,165.7	6.7	<0.1	0.2
Wayne	6,051.7	1.7	<0.1	0.1	
Oklahoma	Alfalfa	2,996.7	182.7	6.1	12.0
	Beaver	15,341.0	23.1	0.2	0.3
	Beckham	4,099.0	108.0	2.6	4.7
	Blaine	3,763.2	203.3	5.4	9.3
	Bryan	5,062.6	10.3	0.2	0.4
	Caddo	24,064.5	25.4	0.1	0.3
	Canadian	5,584.5	441.9	7.9	15.6
	Carter	159,906.5	161.9	0.1	0.5
	Coal	1,193.6	85.9	7.2	21.5

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Oklahoma, cont.	Custer	3,281.4	19.0	0.6	1.2
	Dewey	10,953.7	162.6	1.5	6.2
	Ellis	8,486.3	184.3	2.2	3.2
	Garvin	16,279.0	15.0	0.1	0.4
	Grady	13,537.9	111.5	0.8	2.3
	Grant	5,569.9	77.8	1.4	5.2
	Harper	3,266.8	8.8	0.3	0.4
	Hughes	3,394.5	30.5	0.9	2.2
	Jefferson	4,496.8	<0.1	<0.1	<0.1
	Johnston	1,671.7	32.9	2.0	4.7
	Kay	16,957.9	17.3	0.1	0.4
	Kingfisher	3,744.9	10.2	0.3	0.5
	Kiowa	5,022.4	0.1	<0.1	<0.1
	Latimer	1,062.2	0.6	0.1	0.1
	Le Flore	8,635.9	0.3	<0.1	<0.1
	Logan	4,077.1	4.2	0.1	0.3
	Love	2,011.2	4.4	0.2	0.5
	Major	6,321.8	1.2	<0.1	<0.1
	Marshall	2,613.4	98.4	3.8	7.2
	McClain	2,952.9	2.1	0.1	0.2
Noble	12,990.4	25.3	0.2	1.8	
Oklahoma	47,836.9	1.2	<0.1	<0.1	
Osage	6,971.5	3.8	0.1	0.2	
Pawnee	4,839.9	15.7	0.3	1.4	
Payne	4,332.6	9.9	0.2	0.6	

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Oklahoma, cont.	Pittsburg	6,314.5	349.0	5.5	16.0
	Roger Mills	2,847.0	235.5	8.3	12.6
	Seminole	124,837.3	0.1	<0.1	<0.1
	Stephens	49,990.4	27.7	0.1	0.3
	Texas	110,208.1	0.1	<0.1	<0.1
	Washita	3,310.6	102.1	3.1	5.4
	Woods	4,139.1	155.1	3.7	10.9
Pennsylvania	Allegheny	234,140.2	13.6	<0.1	<0.1
	Armstrong	65,853.3	55.7	0.1	1.8
	Beaver	157,793.2	30.5	<0.1	0.2
	Blair	8,303.8	5.9	0.1	0.2
	Bradford	4,354.5	1,059.4	24.3	78.2
	Butler	5,730.5	121.8	2.1	6.0
	Cameron	292.0	6.6	2.3	4.1
	Centre	16,560.1	38.5	0.2	0.5
	Clarion	1,843.3	8.1	0.4	1.4
	Clearfield	111,051.3	111.5	0.1	2.3
	Clinton	6,161.2	94.4	1.5	3.0
	Columbia	3,810.6	5.6	0.1	0.4
	Crawford	5,091.8	2.4	<0.1	0.1
	Elk	7,876.7	37.5	0.5	1.9
	Fayette	16,465.2	120.2	0.7	2.7
	Forest	744.6	7.7	1.0	1.6
	Greene	13,023.2	359.0	2.8	24.7
Huntingdon	5,121.0	2.7	0.1	0.2	

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Pennsylvania, cont.	Indiana	21,819.7	16.2	0.1	0.7
	Jefferson	1,730.1	13.8	0.8	1.7
	Lawrence	36,598.6	27.0	0.1	1.0
	Lycoming	5,854.6	704.6	12.0	33.8
	McKean	4,723.1	60.5	1.3	4.9
	Potter	2,281.3	16.5	0.7	1.0
	Somerset	10,833.2	5.8	0.1	0.2
	Sullivan	222.7	66.5	29.9	79.8
	Susquehanna	1,617.0	751.3	46.5	123.4
	Tioga	2,909.1	566.3	19.5	47.3
	Venango	2,989.4	2.4	0.1	0.3
	Warren	5,099.1	2.3	<0.1	0.2
	Washington	130,535.0	433.7	0.3	4.6
	Westmoreland	14,607.3	207.0	1.4	3.8
Wyoming	4,788.8	150.0	3.1	15.2	
Texas	Andrews	23,363.7	236.2	1.0	2.7
	Angelina	5,540.7	0.8	<0.1	<0.1
	Archer	2,536.8	0.1	<0.1	<0.1
	Atascosa	15,038.0	327.3	2.2	4.0
	Austin	2,555.0	2.1	0.1	0.1
	Bee	3,087.9	20.0	0.6	1.1
	Borden	2,427.3	8.0	0.3	1.0
	Bosque	3,544.2	0.7	<0.1	<0.1
	Brazos	24,790.8	7.7	<0.1	0.1
	Brooks	1,204.5	1.5	0.1	0.3

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Texas, cont.	Burleson	10,694.5	3.0	<0.1	<0.1
	Cherokee	24,845.6	0.5	<0.1	<0.1
	Clay	1,963.7	<0.1	<0.1	<0.1
	Cochran	24,035.3	3.0	<0.1	<0.1
	Coke	12,713.0	0.3	<0.1	<0.1
	Colorado	52,465.1	0.1	<0.1	<0.1
	Concho	2,832.4	<0.1	<0.1	<0.1
	Cooke	4,533.3	454.3	10.0	29.9
	Cottle	733.7	0.3	<0.1	0.1
	Crane	8,566.6	92.3	1.1	5.7
	Crockett	4,281.5	279.0	6.5	29.5
	Crosby	27,261.9	1.3	<0.1	<0.1
	Culberson	14,311.7	37.7	0.3	0.4
	Dallas	112,204.7	5.6	<0.1	<0.1
	Dawson	28,842.3	17.5	0.1	0.1
	DeWitt	2,394.4	546.6	22.8	48.6
	Denton	60,684.9	455.0	0.7	2.3
	Dimmit	4,073.4	1,794.2	44.0	81.3
	Ector	21,958.4	226.5	1.0	4.6
	Edwards	332.2	<0.1	<0.1	<0.1
	Ellis	8,530.1	4.2	<0.1	0.1
	Erath	5,876.5	0.8	<0.1	<0.1
	Fayette	9,008.2	13.7	0.2	1.2
	Fisher	2,854.3	1.8	0.1	0.1
Franklin	1,956.4	<0.1	<0.1	<0.1	

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Texas, cont.	Freestone	297,861.9	53.9	<0.1	0.5
	Frio	20,589.7	127.5	0.6	0.9
	Gaines	121,778.6	21.6	<0.1	<0.1
	Garza	5,234.1	0.6	<0.1	<0.1
	Glasscock	20,680.9	598.1	2.9	4.2
	Goliad	142,963.2	<0.1	<0.1	<0.1
	Gonzales	7,121.2	577.9	8.1	17.6
	Grayson	8,143.2	9.3	0.1	0.3
	Gregg	33,010.6	9.4	<0.1	0.2
	Grimes	112,500.3	15.5	<0.1	0.3
	Hansford	43,643.1	2.9	<0.1	<0.1
	Hardeman	2,230.2	0.4	<0.1	<0.1
	Hardin	2,376.2	0.1	<0.1	<0.1
	Harrison	11,869.8	141.6	1.2	6.0
	Hartley	113,555.2	1.9	<0.1	<0.1
	Haskell	12,143.6	0.1	<0.1	<0.1
	Hemphill	3,150.0	263.9	8.4	16.3
	Hidalgo	171,630.3	8.0	<0.1	<0.1
	Hockley	46,314.9	3.0	<0.1	<0.1
	Hood	9,351.3	76.0	0.8	2.2
	Houston	3,686.5	8.6	0.2	0.6
	Howard	10,811.3	97.6	0.9	2.7
Hutchinson	34,437.8	0.3	<0.1	<0.1	
Irion	1,335.9	411.4	30.8	74.5	
Jack	2,241.1	14.0	0.6	2.2	

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Texas, cont.	Jefferson	88,585.5	<0.1	<0.1	<0.1
	Jim Hogg	306.6	0.1	<0.1	0.1
	Johnson	9,241.8	582.0	6.3	18.5
	Jones	5,679.4	<0.1	<0.1	<0.1
	Karnes	1,861.5	1,055.2	56.7	120.1
	Kenedy	456.3	0.2	0.1	0.1
	Kent	6,132.0	0.4	<0.1	<0.1
	King	1,485.6	<0.1	<0.1	<0.1
	Kleberg	1,171.7	3.4	0.3	0.5
	Knox	9,800.3	<0.1	<0.1	<0.1
	La Salle	2,474.7	1,288.7	52.1	93.7
	Lavaca	3,763.2	45.0	1.2	2.0
	Lee	3,120.8	1.2	<0.1	0.1
	Leon	2,171.8	56.2	2.6	6.6
	Liberty	20,662.7	<0.1	<0.1	<0.1
	Limestone	11,158.1	10.7	0.1	0.9
	Lipscomb	11,015.7	89.0	0.8	1.1
	Live Oak	1,916.3	294.0	15.3	40.1
	Loving	781.1	138.4	17.7	94.1
	Lynn	19,892.5	1.1	<0.1	<0.1
Madison	1,554.9	45.3	2.9	8.2	
Marion	3,606.2	5.9	0.2	0.9	
Martin	14,063.5	432.0	3.1	4.7	
Maverick	20,498.4	52.4	0.3	0.4	
McMullen	657.0	745.9	113.5	350.4	

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Texas, cont.	Medina	19,228.2	0.2	<0.1	<0.1
	Menard	1,014.7	<0.1	<0.1	<0.1
	Midland	12,891.8	307.4	2.4	3.7
	Milam	16,665.9	4.9	<0.1	0.1
	Mitchell	6,559.1	11.0	0.2	0.3
	Montague	3,989.5	925.3	23.2	77.8
	Montgomery	32,565.3	0.2	<0.1	<0.1
	Moore	57,075.1	<0.1	<0.1	<0.1
	Nacogdoches	5,891.1	271.7	4.6	12.5
	Navarro	18,699.0	4.8	<0.1	0.1
	Newton	2,263.0	0.2	<0.1	<0.1
	Nolan	4,124.5	4.5	0.1	0.2
	Nueces	85,767.7	1.0	<0.1	<0.1
	Ochiltree	21,348.9	33.3	0.2	0.2
	Oldham	2,124.3	1.3	0.1	0.1
	Orange	150,128.2	0.3	<0.1	<0.1
	Palo Pinto	18,403.3	9.6	0.1	0.3
	Panola	6,365.6	346.5	5.4	20.7
	Parker	8,241.7	261.7	3.2	9.8
	Pecos	52,954.2	8.2	<0.1	<0.1
Polk	204,009.5	0.2	<0.1	<0.1	
Potter	2,029.4	0.4	<0.1	<0.1	
Reagan	9,333.1	410.5	4.4	7.8	
Reeves	20,772.2	164.2	0.8	1.1	
Roberts	7,690.6	38.2	0.5	1.2	

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Texas, cont.	Robertson	158,344.3	45.4	<0.1	0.2
	Runnels	2,847.0	<0.1	<0.1	<0.1
	Rusk	582,134.9	65.8	<0.1	0.3
	Sabine	799.4	31.1	3.9	13.9
	San Augustine	1,131.5	182.1	16.1	50.8
	San Patricio	4,172.0	1.1	<0.1	<0.1
	Schleicher	967.3	27.0	2.8	5.0
	Scurry	14,187.6	1.1	<0.1	<0.1
	Shelby	4,920.2	133.6	2.7	8.2
	Sherman	78,073.5	<0.1	<0.1	<0.1
	Smith	11,231.1	0.2	<0.1	<0.1
	Somervell	746,005.3	4.8	<0.1	<0.1
	Starr	9,552.1	5.0	0.1	0.1
	Stephens	13,446.6	2.6	<0.1	0.1
	Sterling	719.1	36.6	5.1	11.9
	Stonewall	923.5	0.9	0.1	0.3
	Sutton	1,153.4	1.6	0.1	0.3
	Tarrant	104,430.2	1,443.0	1.4	3.9
	Terrell	543.9	0.1	<0.1	<0.1
	Terry	48,362.5	7.5	<0.1	<0.1
Tyler	1,872.5	0.1	<0.1	<0.1	
Upshur	8,610.4	0.2	<0.1	<0.1	
Upton	7,975.3	462.6	5.8	14.2	
Van Zandt	4,139.1	0.1	<0.1	<0.1	
Walker	4,478.6	3.4	0.1	0.2	

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Texas, cont.	Waller	9,829.5	0.1	<0.1	<0.1
	Ward	6,909.5	107.3	1.6	4.6
	Washington	2,430.9	2.2	0.1	0.2
	Webb	15,862.9	1,117.8	7.0	18.2
	Wharton	81,606.7	<0.1	<0.1	<0.1
	Wheeler	6,522.6	858.0	13.2	21.5
	Wichita	25,936.9	0.1	<0.1	<0.1
	Wilbarger	12,683.8	0.2	<0.1	<0.1
	Willacy	15,209.6	0.1	<0.1	<0.1
	Wilson	7,843.9	84.5	1.1	1.7
	Winkler	5,274.3	7.7	0.1	0.5
	Wise	24,966.0	529.7	2.1	8.9
	Wood	19,334.1	0.2	<0.1	<0.1
	Yoakum	77,325.3	7.5	<0.1	<0.1
	Young	21,162.7	0.1	<0.1	<0.1
Zapata	2,697.4	1.1	<0.1	0.1	
Zavala	14,410.2	130.0	0.9	1.3	
Utah	Carbon	15,067.2	7.3	<0.1	0.1
	Duchesne	119,811.3	85.5	0.1	0.1
	San Juan	10,632.5	0.3	<0.1	<0.1
	Sevier	52,512.6	<0.1	<0.1	<0.1
	Uintah	100,229.0	157.5	0.2	0.2
Virginia	Buchanan	313.9	0.6	0.2	0.3
	Dickenson	1,741.1	0.8	<0.1	0.2
	Wise	1,927.2	0.1	<0.1	<0.1

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West Virginia	Barbour	773.8	19.9	2.6	6.9
	Brooke	4,551.6	54.8	1.2	5.1
	Doddridge	405.2	78.5	19.4	69.4
	Hancock	28,718.2	1.2	<0.1	<0.1
	Harrison	20,232.0	40.2	0.2	1.9
	Lewis	901.6	2.4	0.3	0.8
	Marion	5,982.4	70.1	1.2	4.9
	Marshall	158,358.9	84.5	0.1	0.7
	Monongalia	42,102.8	6.8	<0.1	0.1
	Ohio	3,825.2	116.5	3.0	10.4
	Pleasants	24,703.2	<0.1	<0.1	<0.1
	Preston	2,890.8	8.4	0.3	1.4
	Ritchie	587.7	2.8	0.5	1.7
	Taylor	824.9	52.9	6.4	17.6
	Tyler	4,934.8	2.1	<0.1	0.2
	Upshur	1,814.1	34.9	1.9	6.8
Webster	1,292.1	2.3	0.2	0.3	
Wetzel	1,467.3	78.2	5.3	11.9	
Wyoming	Big Horn	143,368.4	2.9	<0.1	<0.1
	Campbell	44,318.3	11.7	<0.1	0.1
	Carbon	137,130.5	4.5	<0.1	<0.1
	Converse	56,972.9	106.8	0.2	0.3
	Fremont	186,150.0	28.2	<0.1	<0.1
	Goshen	144,248.0	5.8	<0.1	<0.1
	Hot Springs	28,572.2	0.3	<0.1	<0.1

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State	County	Total annual water use in 2010 (millions of gal) <sup>a</sup>	Annual average hydraulic fracturing water use in 2011 and 2012 (millions of gal) <sup>b</sup>	Hydraulic fracturing water use compared to total water use (%) <sup>c</sup>	Hydraulic fracturing water consumption compared to total water consumption (%) <sup>c,d</sup>
Wyoming, cont.	Johnson	43,205.1	<0.1	<0.1	<0.1
	Laramie	86,297.0	18.3	<0.1	<0.1
	Lincoln	74,562.2	0.8	<0.1	<0.1
	Natrona	62,885.9	1.8	<0.1	<0.1
	Niobrara	25,148.5	0.1	<0.1	<0.1
	Park	111,317.7	0.9	<0.1	<0.1
	Sublette	61,006.1	314.8	0.5	0.7
	Sweetwater	61,699.6	39.4	0.1	0.1
	Uinta	79,518.9	0.6	<0.1	<0.1
	Washakie	60,400.2	1.1	<0.1	<0.1

<sup>a</sup> County-level data accessed from the USGS website (<http://water.usgs.gov/watuse/data/2010/>) on November 11, 2014. Total daily water withdrawals were multiplied by 365 days to estimate total water use for the year ([Maupin et al., 2014](#)).

<sup>b</sup> Average of water used for hydraulic fracturing in 2011 and 2012, as reported to FracFocus ([U.S. EPA, 2015c](#)).

<sup>c</sup> Percentages were calculated by averaging annual water use for hydraulic fracturing reported in FracFocus in 2011 and 2012 for a given county ([U.S. EPA, 2015c](#)), and then dividing by 2010 USGS total water use for that county ([Maupin et al., 2014](#)) and multiplying by 100.

<sup>d</sup> Consumption values were calculated with use-specific consumption rates predominantly from the USGS, including 19.2% for public supply, 19.2% for domestic use, 60.7% for irrigation, 60.7% for livestock, 14.8% for industrial uses, 14.8% for mining ([Solley et al., 1998](#)), and 2.7% for thermoelectric power ([USGS, 2014](#)). We used a rate of 71.6% for aquaculture ([from Verdegem and Bosma, 2009](#)) (evaporation per kg fish + infiltration per kg)/(total water use per kg)\*100. These rates were multiplied by each USGS water use value ([Maupin et al., 2014](#)) to yield a total water consumption estimate. To calculate a consumption amount for hydraulic fracturing, we used a consumption rate of 82.5%. This was calculated by taking the median value for all reported produced water/injected water percentages in Tables 7-1 and 7-2 of this assessment and then subtracting from 100%. If a range of values was given, the midpoint was used. Note that this is likely a low estimate of consumption since much of this return water is not subsequently treated and reused, but rather disposed of in underground injection wells—see Chapter 8.

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**Table B-3. Comparison of water use per well estimates from the EPA’s project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) and literature sources.**Source: ([U.S. EPA, 2015c](#))

State	Basin <sup>a</sup>	Water use per well (gal) - FracFocus estimate <sup>b</sup>	Water use per well (gal) - Literature estimate <sup>b,c</sup>	FracFocus estimate as a percentage of literature estimate (%)
Colorado	Denver	403,686	2,900,000	14
North Dakota		2,140,842	2,200,000	97
Oklahoma		2,591,778	3,000,000	86
Pennsylvania <sup>d</sup>		4,301,701	4,450,000	97
Texas	Fort Worth	3,881,220	4,500,000	86
Texas	Salt	3,139,980	4,000,000	78
Texas	Western Gulf	3,777,648	4,600,000	82
Average <sup>e</sup>				77
Median <sup>e</sup>				86

<sup>a</sup> In cases where a basin is not specified, estimates were for the entire state and not specific to a particular basin. Basin boundaries for the FracFocus estimates were determined from data from the U.S. EIA ([see U.S. EPA, 2015b](#)).

<sup>b</sup> The type of literature estimate determined the specific comparison with FracFocus. If averages were given in the literature (as for North Dakota and Pennsylvania), those values were compared with FracFocus averages; where medians were given in the literature (as for Colorado, Oklahoma, and Texas), they were compared with FracFocus medians.

<sup>c</sup> Literature estimates were from the following sources: Colorado ([Goodwin et al., 2014](#)), North Dakota ([North Dakota State Water Commission, 2014](#)), Pennsylvania ([Mitchell et al., 2013](#)), and Texas ([Nicot et al., 2012](#))—see far right-column and footnotes in Table B-5 for details on literature estimates. Where the literature provided a range, the mid-point was used. Only literature estimates that were not directly derived from FracFocus were included.

<sup>d</sup> The results from [Mitchell et al. \(2013\)](#) were used for Pennsylvania since they were derived from Pennsylvania Department of Environment Protection records. Estimates from [Hansen et al. \(2013\)](#) were not included here because they were based on FracFocus.

<sup>e</sup> Average and median percentage calculations were not weighted by the number of wells for a given estimate.

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**Table B-4. Comparison of well counts from the EPA’s project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) and state databases for North Dakota, Pennsylvania, and West Virginia.**

State	FracFocus well counts <sup>a</sup>			State database well counts			FracFocus counts as a percentage of state database counts		
	2011	2012	Total	2011	2012	Total	2011	2012	Total
North Dakota <sup>b</sup>	613	1,458	2,071	1,225	1,740	2,965	50%	84%	70%
Pennsylvania <sup>c</sup>	1,137	1,257	2,394	1,963	1,347	3,310	58%	93%	72%
West Virginia <sup>d</sup>	93	176	269	214	251	465	43%	70%	58%
Average							50%	82%	67%

<sup>a</sup> FracFocus disclosures from [U.S. EPA \(2015c\)](#).

<sup>b</sup> For North Dakota state well counts, we used a North Dakota Department of Mineral Resources online database containing a list of horizontal wells completed in the Bakken Formation. Data for North Dakota were accessed on July 9, 2014 at <https://www.dmr.nd.gov/oilgas/bakkenwells.asp>.

<sup>c</sup> For Pennsylvania state well counts, we used completed horizontal wells as a proxy for hydraulically fractured wells in the state. The Pennsylvania Department of Environmental Protection has online databases of permitted and spudded wells, which differentiate between conventional and unconventional wells and can generate summary statistics at both the county and state scale. The number of spudded wells (i.e., wells drilled) provided a better comparison with the number of hydraulically fractured wells in FracFocus than that of permitted wells. The number of permitted wells was nearly double that of spudded in 2011 and 2012, indicating that almost half of the wells permitted were not drilled in that same year. Therefore, we used spudded wells here. Data for Pennsylvania were accessed on February 11, 2014 from [http://www.depreportingservices.state.pa.us/ReportServer/Pages/ReportViewer.aspx?/Oil\\_Gas/Spud\\_External\\_Data](http://www.depreportingservices.state.pa.us/ReportServer/Pages/ReportViewer.aspx?/Oil_Gas/Spud_External_Data).

<sup>d</sup> For West Virginia state well counts, data on the number of hydraulically fractured wells per year were received from the West Virginia Department of Environmental Protection on February 25, 2014.

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**Table B-5. Water use per hydraulically fractured well as reported in the EPA’s project database of disclosures to FracFocus 1.0 (U.S. EPA, 2015c) by state and basin.**

Source: ([U.S. EPA, 2015c](#))

Other literature estimates are also included where available. NA indicates other literature estimates were not available. All FracFocus estimates were limited to disclosures with valid state, county, and volume information. States listed in order addressed in Chapter 4.

State	Basin/total <sup>a</sup>	Number of disclosures	Mean (gal)	Median (gal)	10 <sup>th</sup> percentile (gal)	90 <sup>th</sup> percentile (gal)	Literature estimates
Texas	Permian	8,419	1,068,511	841,134	40,090	1,814,633	Many formations reported <sup>b</sup>
	Western Gulf	4,549	3,915,540	3,777,648	173,832	6,786,052	4.5–4.7 million gal (median, Eagle Ford play) <sup>b</sup>
	Fort Worth	2,564	3,880,724	3,881,220	923,381	6,649,406	4.5 million gal (median, Barnett play) <sup>b</sup>
	TX-LA-MS Salt	626	4,261,363	3,139,980	193,768	10,010,707	6–7.5 million gal (median, Texas-Haynesville play) and 0.5-1 million gallons (median, Cotton Valley play) <sup>b</sup>
	Anadarko	604	4,128,702	3,341,310	492,421	8,292,996	Many formations reported <sup>b</sup>
	Other	120	1,601,897	184,239	21,470	5,678,588	NA
	Total	16,882	2,494,452	1,420,613	58,709	6,115,195	Not reported by state <sup>b</sup>
Colorado	Denver	3,166	753,887	403,686	143,715	2,588,946	2.9 million gal (median, Wattenberg field of Niobrara play) <sup>c</sup>
	Uinta-Piceance	1,520	2,739,523	1,798,414	840,778	5,066,380	NA
	Raton	146	108,003	95,974	24,917	211,526	NA
	Other	66	605,740	183,408	34,412	601,816	NA
	Total	4,898	1,348,842	463,462	147,353	3,092,024	NA

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State	Basin/total <sup>a</sup>	Number of disclosures	Mean (gal)	Median (gal)	10 <sup>th</sup> percentile (gal)	90 <sup>th</sup> percentile (gal)	Literature estimates
Wyoming	Greater Green River	861	841,702	752,979	147,020	1,493,266	NA
	Powder River	351	739,129	5,927	5,353	2,863,182	NA
	Other	193	613,618	41,664	22,105	1,818,606	NA
	Total	1,405	784,746	322,793	5,727	1,837,602	NA
Pennsylvania	Appalachian	2,445	4,301,701	4,184,936	2,313,649	6,615,981	4.2-4.6 million gal (average, Marcellus play, Susquehanna River Basin) <sup>d</sup>
	Total	2,445	4,301,701	4,184,936	2,313,649	6,615,981	4.1-4.5 <sup>d</sup> and 4.3-4.6 <sup>e</sup> million gal (average)
West Virginia	Appalachian	273	5,034,217	5,012,238	3,170,210	7,297,080	NA
	Total	273	5,034,217	5,012,238	3,170,210	7,297,080	4.7-6 million gal (average) <sup>d</sup>
Ohio	Appalachian	146	4,206,955	3,887,499	2,885,568	5,571,027	NA
	Total	146	4,206,955	3,887,499	2,885,568	5,571,027	NA
North Dakota	Williston	2,109	2,140,842	2,022,380	969,380	3,313,482	NA
	Total	2,109	2,140,842	2,022,380	969,380	3,313,482	2.2 million gal (average) <sup>f</sup>
Montana	Williston	187	1,640,085	1,552,596	375,864	3,037,398	NA
	Other	20	945,541	1,017,701	157,639	1,575,197	NA
	Total	207	1,572,979	1,455,757	367,326	2,997,552	NA
Oklahoma	Anadarko	935	3,742,703	3,259,774	1,211,700	6,972,652	Many formations reported <sup>g</sup>
	Arkoma	158	6,323,750	6,655,929	172,375	9,589,554	Many formations reported <sup>g</sup>
	Ardmore	98	6,637,332	8,021,559	81,894	8,835,842	Many formations reported <sup>g</sup>
	Other	592	1,963,480	1,866,144	1,319,247	2,785,352	NA
	Total	1,783	3,539,775	2,591,778	1,260,906	7,402,230	3 million gal (median) <sup>g</sup>

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State	Basin/total <sup>a</sup>	Number of disclosures	Mean (gal)	Median (gal)	10 <sup>th</sup> percentile (gal)	90 <sup>th</sup> percentile (gal)	Literature estimates
Kansas	Total	121	1,135,973	1,453,788	10,836	2,227,926	NA
Arkansas	Arkoma	1,423	5,190,254	5,259,965	3,234,963	7,121,249	NA
	Total	1,423	5,190,254	5,259,965	3,234,963	7,121,249	NA
Louisiana	TX-LA-MS Salt	939	5,289,100	5,116,650	2,851,654	7,984,838	NA
	Other	27	896,899	232,464	87,003	3,562,400	NA
	Total	966	5,166,337	5,077,863	1,812,099	7,945,630	NA
Utah	Uinta-Piceance	1,396	375,852	304,105	77,166	770,699	NA
	Other	10	58,874	56,245	28,745	97,871	NA
	Total	1,406	373,597	302,075	76,286	769,360	NA
New Mexico	Permian	732	991,369	426,258	89,895	2,502,923	NA
	San Juan	363	159,680	97,734	27,217	313,919	NA
	Other	50	33,787	8,358	1,100	98,841	NA
	Total	1,145	685,882	175,241	35,638	1,871,666	NA

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State	Basin/total <sup>a</sup>	Number of disclosures	Mean (gal)	Median (gal)	10 <sup>th</sup> percentile (gal)	90 <sup>th</sup> percentile (gal)	Literature estimates
California	San Joaquin	677	131,653	77,238	22,100	285,029	NA
	Other	34	132,391	36,099	13,768	361,192	NA
	Total	711	131,689	76,818	21,462	285,306	130,000 gallon (average) <sup>h</sup>

<sup>a</sup> Basin boundaries for the FracFocus estimates were determined from data from the U.S. EIA ([see U.S. EPA, 2015b](#)).

<sup>b</sup> Literature estimates for Texas were from [Nicot et al. \(2012\)](#), using proprietary data from IHS. In most cases, Nicot et al. reported at the play scale or smaller, rather than the EIA basin scale used for FracFocus. We reference 2011 and 2012 (partial year) for Nicot et al. where possible to overlap with the period of study for FracFocus, though more years were available for most formations. A range is reported for some medians because median water use was different for the two years. There were five formations reported for the Permian Basin (Wolfberry, Wolfcamp, Canyon, Clearfork, and San Andres-Greyburg). The most active area in the Permian Basin in 2011–2012 was the Wolfberry, which reported a median of 1 to 1.1 million gallons per well—these were mostly vertical wells. For the TX-LA-MS Salt Basin, Nicot et al. reported two formations (TX-Haynesville and Cotton Valley), with similar levels of activity in 2011-2012. Wells in TX-Haynesville were predominantly horizontal, while those in Cotton Valley were predominantly vertical (though horizontal wells in Cotton Valley were also reported). There were three fields reported in the Anadarko Basin (Granite Wash, Cleveland, and Marmaton). The most active area in the Anadarko Basin in 2011-2012 was the Granite Wash, which reported a median of 3.3 to 5.2 million gallons per well and where wells were mostly horizontal.

<sup>c</sup> Literature estimates for the Denver Basin were from [Goodwin et al. \(2014\)](#). Goodwin et al. assessed 200 randomly sampled wells in the Wattenberg Field of the Denver Basin (Niobrara Play), using industry data for wells operated by Noble Energy, drilled between January 1, 2010, and July 1, 2013. Water consumption is reported rather than water use, but Goodwin et al. assume, based on Noble Energy practices, that water use and water consumption were identical because none of the flowback or produced water is reused for hydraulic fracturing. Goodwin et al. reported drilling water consumed, hydraulic fracturing water consumed, and total water consumed. We present hydraulic fracturing water consumption here (hydraulic fracturing water consumption was approximately 95% of the total).

<sup>d</sup> [Hansen et al. \(2013\)](#), using data from FracFocus via Skytruth. For the Susquehanna River Basin portion of the Marcellus play, and for Pennsylvania as a whole, the range of annual averages is reported for 2011 and 2012. Similarly, for West Virginia, the range of annual averages is reported for 2011 and 2012 (partial year).

<sup>e</sup> [Mitchell et al. \(2013\)](#), using data reported to the Pennsylvania Department of Environmental Protection. Mitchell et al. reported water use in the Ohio River Basin for 2011 and 2012 (partial year) for horizontal and vertical wells. Here we report results for horizontal wells, which made up the majority of wells over the two-year period (i.e., 93%, 1,191 horizontal wells versus 96 vertical wells). A range is reported as before because the average water use differed between the two years.

<sup>f</sup> Literature estimates for North Dakota were from an informational bulletin from the [North Dakota State Water Commission \(2014\)](#). No further information was available.

<sup>g</sup> [Murray \(2013\)](#), who assessed water use for oil and gas operations from 2000–2010 for eight formations in Oklahoma using data from the Oklahoma Corporation Commission. It is not possible to extract an estimate corresponding to 2011–2012 from Murray without the raw data, because medians were presented for the 10-year period rather than separated by year.

<sup>h</sup> Literature estimates for California were from a California Council on Science and Technology report using data from FracFocus ([CCST, 2014](#)).

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**Table B-6. Estimated percent domestic use water from ground water and self-supplied by county.**

Counties listed contained hydraulically fractured wells with valid state, county, and volume information (U.S. EPA, 2015c).

Data estimated from the USGS Water Census (Maupin et al., 2014).

State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Alabama	Jefferson	11.9	0.8
	Tuscaloosa	10.7	6.1
Arkansas	Cleburne	0.0	0.0
	Conway	8.6	8.6
	Faulkner	48.0	3.5
	Independence	20.5	9.4
	Logan	0.0	0.0
	Sebastian	0.0	0.0
	Van Buren	6.4	6.4
	White	0.4	0.0
	Yell	1.8	1.8
California	Colusa	97.9	10.3
	Glenn	96.5	21.6
	Kern	74.5	1.7
	Los Angeles	45.0	4.2
	Sutter	19.4	4.6
	Ventura	30.9	3.9
Colorado	Adams	18.1	2.8
	Arapahoe	19.3	1.3
	Boulder	1.7	1.5
	Broomfield	0.0	0.0
	Delta	59.6	28.4
	Dolores	55.2	51.4
	El Paso	19.6	5.1
	Elbert	100.0	75.2
	Fremont	15.6	15.6

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Colorado, cont.	Garfield	36.7	28.5
	Jackson	84.4	40.7
	La Plata	24.4	11.3
	Larimer	2.3	0.8
	Las Animas	26.3	16.0
	Mesa	7.3	6.2
	Moffat	36.4	25.8
	Morgan	57.9	4.9
	Phillips	100.0	25.3
	Rio Blanco	60.2	32.5
	Routt	22.6	5.9
	San Miguel	71.4	32.5
	Weld	4.7	0.7
	Yuma	100.0	38.1
Kansas	Barber	100.0	19.0
	Clark	100.0	24.2
	Comanche	100.0	19.2
	Finney	100.0	2.1
	Grant	100.0	23.8
	Gray	100.0	36.4
	Harper	100.0	10.3
	Haskell	100.0	35.2
	Hodgeman	100.0	42.3
	Kearny	100.0	14.6
	Lane	100.0	24.1
	Meade	100.0	25.4
	Morton	100.0	21.7
	Ness	100.0	24.2
Seward	100.0	15.7	

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Kansas, cont.	Sheridan	100.0	44.9
	Stanton	100.0	29.8
	Stevens	100.0	25.9
	Sumner	51.3	0.0
Louisiana	Allen	100.0	7.5
	Beauregard	100.0	20.6
	Bienville	100.0	16.8
	Bossier	29.4	14.6
	Caddo	12.2	8.8
	Calcasieu	98.3	12.7
	Caldwell	100.0	6.5
	Claiborne	100.0	10.4
	De Soto	55.8	21.8
	East Feliciana	100.0	11.8
	Jackson	100.0	13.8
	Lincoln	100.0	4.2
	Natchitoches	23.2	11.4
	Rapides	100.0	3.3
	Red River	83.2	27.6
	Sabine	67.5	36.2
	Tangipahoa	100.0	26.9
	Union	100.0	11.2
	Webster	100.0	11.3
	West Feliciana	100.0	2.4
Winn	100.0	16.4	
Michigan	Cheboygan	100.0	76.4
	Gladwin	100.0	84.5
	Kalkaska	100.0	89.0
	Missaukee	100.0	90.6
	Ogemaw	100.0	90.8
	Roscommon	100.0	91.9

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Mississippi	Amite	100.0	26.0
	Wilkinson	100.0	11.1
Montana	Daniels	100.0	29.4
	Garfield	100.0	70.0
	Glacier	62.1	17.7
	Musselshell	89.9	54.5
	Richland	100.0	30.8
	Roosevelt	84.2	20.9
	Rosebud	51.3	10.3
	Sheridan	100.0	31.0
New Mexico	Chaves	100.0	11.8
	Colfax	30.7	2.6
	Eddy	100.0	2.2
	Harding	100.0	25.0
	Lea	100.0	17.4
	Rio Arriba	84.0	42.3
	Roosevelt	100.0	8.9
	San Juan	14.6	12.9
	Sandoval	98.9	23.2
North Dakota	Billings	NA	33.3
	Bottineau	100.0	13.7
	Burke	100.0	12.5
	Divide	100.0	12.5
	Dunn	100.0	21.4
	Golden Valley	100.0	7.7
	Mckenzie	75.8	15.7
	Mclean	12.5	9.9
	Mountrail	65.7	11.5
	Stark	NA	5.7
	Williams	27.4	7.3

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Ohio	Ashland	98.8	57.4
	Belmont	76.4	8.9
	Carroll	96.4	76.4
	Columbiana	63.2	43.2
	Coshocton	99.3	34.9
	Guernsey	37.6	9.5
	Harrison	65.6	45.9
	Jefferson	33.1	10.2
	Knox	99.2	41.1
	Medina	98.4	83.1
	Muskingum	93.4	17.0
	Noble	8.0	8.0
	Portage	32.6	18.3
	Stark	91.2	30.9
	Tuscarawas	94.0	23.5
Wayne	99.1	49.0	
Oklahoma	Alfalfa	100.0	14.6
	Beaver	100.0	47.9
	Beckham	100.0	10.6
	Blaine	100.0	8.8
	Bryan	26.0	7.8
	Caddo	45.4	35.1
	Canadian	100.0	0.0
	Carter	17.5	0.5
	Coal	31.5	27.5
	Custer	70.8	13.2
	Dewey	100.0	22.5
	Ellis	100.0	31.4
	Garvin	41.3	15.8
	Grady	100.0	34.2
	Grant	100.0	13.2
Harper	100.0	22.6	

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Oklahoma, cont.	Hughes	23.6	6.7
	Jefferson	13.5	1.8
	Johnston	53.4	1.1
	Kay	39.2	4.6
	Kingfisher	100.0	28.3
	Kiowa	10.3	0.0
	Latimer	12.6	12.6
	Le Flore	14.3	13.1
	Logan	61.1	34.6
	Love	100.0	3.8
	Major	100.0	28.1
	Marshall	20.1	4.4
	McClain	95.9	23.9
	Noble	23.3	14.3
	Oklahoma	22.0	2.5
	Osage	18.0	14.9
	Pawnee	38.2	27.7
	Payne	47.9	12.6
	Pittsburg	0.6	0.0
	Roger Mills	80.1	19.4
Seminole	78.8	16.1	
Stephens	99.2	14.9	
Texas	100.0	10.9	
Washita	53.9	18.2	
Woods	100.0	14.7	
Pennsylvania	Allegheny	15.7	15.3
	Armstrong	45.3	36.8
	Beaver	54.7	26.8
	Blair	34.9	24.0
	Bradford	100.0	65.2
	Butler	51.8	42.8
	Cameron	29.0	29.0

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Pennsylvania, cont.	Centre	93.1	21.3
	Clarion	61.5	55.8
	Clearfield	38.4	22.7
	Clinton	48.4	38.1
	Columbia	77.5	56.7
	Crawford	97.7	66.0
	Elk	25.3	15.6
	Fayette	19.2	16.1
	Forest	100.0	78.3
	Greene	31.9	31.9
	Huntingdon	73.2	57.8
	Indiana	52.2	49.1
	Jefferson	60.7	46.1
	Lawrence	40.5	38.8
	Lycoming	60.0	29.3
	McKean	56.6	33.3
	Potter	93.7	58.1
	Somerset	42.6	33.5
	Sullivan	100.0	76.9
	Susquehanna	79.9	74.7
	Tioga	81.3	58.3
Venango	95.9	32.7	
Warren	96.9	49.4	
Washington	21.6	21.5	
Westmoreland	21.3	19.8	
Wyoming	100.0	70.6	
Texas	Andrews	100.0	23.4
	Angelina	100.0	9.8
	Archer	16.9	16.9
	Atascosa	100.0	16.3
	Austin	100.0	55.6
	Bee	100.0	52.5

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Texas, cont.	Borden	100.0	71.4
	Bosque	88.7	30.3
	Brazos	100.0	2.1
	Brooks	100.0	35.3
	Burleson	100.0	42.9
	Cherokee	87.5	26.1
	Clay	44.6	36.7
	Cochran	100.0	23.3
	Coke	29.0	28.9
	Colorado	100.0	45.4
	Concho	96.8	5.0
	Cooke	75.5	8.9
	Cottle	100.0	21.4
	Crane	100.0	14.3
	Crockett	100.0	42.5
	Crosby	35.6	19.0
	Culberson	100.0	13.8
	Dallas	1.0	0.7
	Dawson	100.0	33.8
	DeWitt	100.0	42.3
	Denton	9.0	3.6
	Dimmit	100.0	30.5
	Ector	100.0	28.3
	Edwards	100.0	42.1
	Ellis	32.2	7.9
	Erath	100.0	43.3
	Fayette	100.0	27.6
	Fisher	NA	36.8
	Franklin	0.9	0.0
	Freestone	100.0	31.2
Frio	100.0	20.4	
Gaines	100.0	45.5	

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Texas, cont.	Garza	20.1	17.2
	Glasscock	NA	100.0
	Goliad	NA	66.7
	Gonzales	96.8	15.9
	Grayson	56.0	4.2
	Gregg	20.8	14.1
	Grimes	100.0	26.0
	Hansford	100.0	16.4
	Hardeman	87.6	13.3
	Hardin	100.0	29.5
	Harrison	43.8	24.8
	Hartley	100.0	39.7
	Haskell	100.0	15.7
	Hemphill	100.0	27.5
	Hidalgo	9.2	1.6
	Hockley	100.0	27.4
	Hood	70.8	39.8
	Houston	79.7	36.6
	Howard	100.0	19.8
	Hutchinson	27.3	14.9
	Irion	100.0	50.0
	Jack	46.7	43.8
	Jefferson	25.0	5.8
	Jim Hogg	NA	25.0
	Johnson	34.9	6.8
	Jones	60.5	60.5
	Karnes	100.0	17.6
	Kenedy	100.0	25.0
	Kent	100.0	37.5
	King	100.0	33.3
Kleberg	100.0	1.9	
Knox	86.2	24.2	

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Texas, cont.	La Salle	100.0	43.3
	Lavaca	100.0	56.0
	Lee	100.0	15.9
	Leon	100.0	41.4
	Liberty	98.5	42.5
	Limestone	46.5	32.5
	Lipscomb	100.0	23.5
	Live Oak	32.8	32.1
	Loving	NA	0.0
	Lynn	64.1	32.2
	Madison	100.0	66.9
	Marion	13.7	8.4
	Martin	100.0	48.9
	Maverick	27.6	27.6
	McMullen	100.0	40.0
	Medina	98.0	23.6
	Menard	36.4	36.4
	Midland	100.0	22.1
	Milam	82.5	41.1
	Mitchell	100.0	14.7
	Montague	57.1	49.7
	Montgomery	100.0	26.6
	Moore	100.0	8.1
	Nacogdoches	55.6	21.6
	Navarro	22.0	22.0
	Newton	100.0	63.7
	Nolan	100.0	17.6
	Nueces	5.6	5.6
	Ochiltree	100.0	16.8
	Oldham	100.0	58.8
Orange	99.1	41.2	
Palo Pinto	11.7	11.7	

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Texas, cont.	Panola	96.6	58.7
	Parker	63.5	41.1
	Pecos	100.0	31.3
	Polk	41.9	41.7
	Potter	100.0	12.6
	Reagan	100.0	16.2
	Reeves	100.0	31.1
	Roberts	100.0	33.3
	Robertson	97.1	22.5
	Runnels	13.5	13.5
	Rusk	90.7	41.8
	Sabine	76.2	69.0
	San Augustine	78.0	74.4
	San Patricio	88.8	21.8
	Schleicher	100.0	40.0
	Scurry	32.5	27.7
	Shelby	66.2	58.2
	Sherman	100.0	33.3
	Smith	48.0	13.7
	Somervell	87.7	69.3
	Starr	23.2	23.2
	Stephens	13.5	13.5
	Sterling	NA	18.8
	Stonewall	NA	40.0
	Sutton	100.0	26.7
	Tarrant	3.7	1.3
	Terrell	100.0	25.0
	Terry	100.0	16.7
Tyler	100.0	73.6	
Upshur	54.1	23.2	
Upton	100.0	15.2	
Van Zandt	65.7	39.0	

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Texas, cont.	Walker	57.7	30.6
	Waller	100.0	37.2
	Ward	100.0	4.5
	Washington	48.2	36.0
	Webb	99.4	0.5
	Wharton	100.0	45.9
	Wheeler	100.0	31.3
	Wichita	8.8	2.9
	Wilbarger	100.0	11.5
	Willacy	28.4	28.4
	Wilson	100.0	6.9
	Winkler	100.0	3.8
	Wise	51.3	50.4
	Wood	21.3	12.9
	Yoakum	100.0	36.0
	Young	19.3	18.9
Zapata	13.9	13.9	
Zavala	100.0	15.2	
Utah	Carbon	50.0	1.2
	Duchesne	57.1	10.4
	San Juan	68.3	47.5
	Sevier	100.0	10.0
	Uintah	87.7	3.1
Virginia	Buchanan	NA	27.6
	Dickenson	2.5	2.5
	Wise	5.9	2.3
West Virginia	Barbour	24.1	24.8
	Brooke	33.4	6.8
	Doddridge	60.6	62.1
	Hancock	67.7	6.9
	Harrison	8.8	8.9
	Lewis	29.5	30.3

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
West Virginia, cont.	Marion	5.8	4.9
	Marshall	96.5	12.0
	Monongalia	5.3	5.5
	Ohio	5.4	3.4
	Pleasants	100.0	27.9
	Preston	66.1	41.0
	Ritchie	45.2	46.4
	Taylor	14.9	14.9
	Tyler	44.4	39.2
	Upshur	27.3	27.8
	Webster	41.9	43.2
	Wetzel	96.3	28.6
Wyoming	Big Horn	79.4	11.3
	Campbell	100.0	0.6
	Carbon	63.8	6.7
	Converse	96.5	17.0
	Fremont	49.3	23.7
	Goshen	100.0	21.1
	Hot Springs	31.9	8.2
	Johnson	40.8	35.4
	Laramie	38.1	13.0
	Lincoln	82.4	9.0
	Natrona	69.0	6.6
	Niobrara	100.0	16.3
	Park	18.9	13.7

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State	County	Percent domestic use water from ground water <sup>a,b</sup>	Percent domestic use water self supplied <sup>a,c</sup>
Wyoming, cont.	Sublette	54.6	22.1
	Sweetwater	3.5	0.4
	Uinta	19.5	11.5
	Washakie	100.0	16.0

<sup>a</sup> Data accessed from the USGS website (<http://water.usgs.gov/watuse/data/2010/>) on November 11, 2014. Domestic water use is water used for indoor household purposes such as drinking, food preparation, bathing, washing clothes and dishes, flushing toilets, and outdoor purposes such as watering lawns and gardens (Maupin et al., 2014).

<sup>b</sup> Percent domestic water use from ground water estimated with the following equation: (Domestic public supply volume from ground water + Domestic self-supplied volume from ground water) / Domestic total water use volume \* 100. Domestic public supply volume from ground water was estimated by multiplying the volume of domestic water from public supply by the ratio of public supply volume from ground water to total public supply volume.

<sup>c</sup> Percent domestic water use self-supplied estimated by dividing the volume of domestic water self-supplied by total domestic water use volume.

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**Table B-7. Projected hydraulic fracturing water use by Texas counties between 2015 and 2060, expressed as a percentage of 2010 total county water use.**

Hydraulic fracturing water use data from [Nicot et al. \(2012\)](#). Total water use data from 2010 from the USGS Water Census ([Maupin et al., 2014](#)). All 254 Texas counties are listed by descending order of percentages in 2030.

Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
McMullen	126.2	137.0	152.1	165.1	176.7	164.0	145.3	126.6	108.0	89.3
Irion	36.1	59.2	70.5	63.7	53.4	43.1	32.8	22.4	12.1	5.4
La Salle	58.4	58.3	59.7	60.8	61.9	54.6	45.3	36.0	26.7	17.4
San Augustine	60.2	56.2	52.2	48.2	44.2	40.2	36.2	32.1	28.1	24.1
Sterling	12.0	32.0	39.9	40.5	41.0	34.7	28.3	21.9	15.6	10.7
Dimmit	38.2	38.1	38.9	39.0	38.7	33.9	27.9	22.0	16.0	10.1
Sabine	9.6	19.2	28.7	38.3	35.1	31.9	28.7	25.6	22.3	19.2
Leon	9.9	19.3	27.0	34.6	32.9	29.0	25.1	21.2	17.3	13.5
Karnes	48.1	43.0	37.9	32.6	27.2	21.8	16.4	11.0	5.6	0.2
Loving	13.1	17.4	23.4	29.4	28.8	26.2	23.6	20.9	18.3	15.7
Shackelford	0.0	7.9	15.7	23.6	21.2	18.9	16.5	14.1	11.8	9.4
Madison	5.5	11.8	15.7	19.7	17.4	15.2	13.0	10.9	8.7	6.5
Schleicher	10.5	15.8	19.1	19.7	17.1	14.5	11.9	9.3	6.7	4.7
Sutton	0.0	11.0	15.1	19.1	23.2	20.6	18.1	15.5	12.9	10.3
Shelby	11.0	20.4	19.4	18.4	17.4	15.7	14.1	12.5	10.9	9.3
DeWitt	26.9	24.1	21.4	18.4	15.4	12.3	9.3	6.3	3.2	0.2
Hemphill	25.7	23.1	20.5	17.8	15.2	12.6	10.0	7.3	4.7	2.1

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Terrell	0.0	9.7	13.2	16.8	20.4	18.2	15.9	13.6	11.3	9.0
Coryell	7.0	24.4	22.8	16.5	10.1	3.8	0.0	0.0	0.0	0.0
Montague	28.6	24.5	20.4	16.3	12.2	8.2	4.1	0.0	0.0	0.0
Crockett	7.6	12.5	14.8	13.4	11.2	9.1	6.9	4.7	2.5	1.1
Upton	12.1	15.2	14.1	12.9	11.7	9.8	7.9	5.9	4.0	2.7
Borden	3.1	8.6	12.0	12.1	12.2	10.3	8.4	6.4	4.5	3.1
Live Oak	13.3	12.4	11.5	11.8	12.2	12.7	13.2	11.7	9.8	7.8
Reagan	11.2	14.0	12.7	11.3	9.9	8.1	6.4	4.6	2.8	1.6
Clay	3.2	5.9	8.6	11.3	10.3	9.4	8.4	7.5	6.6	5.6
Wheeler	17.6	15.3	13.1	10.8	8.6	6.3	4.1	1.8	0.0	0.0
Lavaca	7.9	13.2	12.0	10.7	9.4	8.1	6.7	5.4	4.0	2.7
Washington	0.0	6.7	11.8	10.7	9.6	8.6	7.5	6.4	5.3	4.3
Nacogdoches	7.9	11.4	10.7	10.0	9.2	8.3	7.5	6.6	5.7	4.9
Hill	17.1	14.7	12.2	9.8	7.3	4.9	2.4	0.0	0.0	0.0
Jack	3.5	5.3	7.1	8.8	7.9	7.1	6.2	5.3	4.4	3.5
Panola	7.2	10.2	9.2	8.5	7.7	7.0	6.3	5.5	4.8	4.0
Jim Hogg	4.8	6.4	8.0	8.0	6.9	6.0	4.9	3.9	2.9	1.8
Howard	4.4	7.1	8.5	8.0	6.8	5.6	4.4	3.2	2.1	1.3
Parker	3.7	5.0	6.3	7.6	6.8	6.1	5.3	4.5	3.8	3.0
Hamilton	8.8	10.7	8.9	7.1	5.3	3.5	1.8	0.0	0.0	0.0
Johnson	14.2	11.9	9.5	7.1	4.7	2.4	0.0	0.0	0.0	0.0
Midland	6.7	8.3	7.7	7.1	6.2	5.2	4.1	3.0	2.0	1.2

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Kenedy	4.1	5.4	6.8	6.8	5.9	5.1	4.1	3.3	2.4	1.6
Fayette	3.9	8.4	7.6	6.6	5.5	4.4	3.4	2.3	1.2	0.2
Lee	2.1	4.1	5.3	6.5	5.8	5.1	4.3	3.6	2.9	2.1
Winkler	2.9	3.8	5.1	6.3	6.0	5.4	4.7	4.1	3.4	2.8
Wilson	6.7	7.7	7.0	6.2	5.4	4.6	3.9	3.1	2.3	1.5
Martin	5.7	7.1	6.5	6.0	5.3	4.4	3.5	2.6	1.8	1.2
Burleson	1.0	2.9	4.3	5.7	5.1	4.5	3.9	3.3	2.6	2.0
Atascosa	6.3	5.7	5.6	5.6	5.6	5.6	5.0	4.2	3.4	2.7
Bosque	1.8	3.0	4.3	5.5	5.1	4.6	4.2	3.7	3.2	2.8
Webb	7.5	7.1	6.3	5.4	4.6	3.8	3.1	2.3	1.4	0.5
Gonzales	8.0	7.1	6.2	5.3	4.4	3.6	2.7	1.8	0.9	0.0
Marion	1.1	2.4	3.8	5.1	5.2	4.7	4.2	3.7	3.2	2.7
Harrison	4.3	6.1	5.5	5.1	4.6	4.2	3.7	3.3	2.9	2.4
Eastland	0.0	3.9	5.9	5.0	4.2	3.3	2.5	1.7	0.8	0.0
Archer	1.0	2.4	3.6	4.9	4.5	4.1	3.7	3.3	2.9	2.5
Zavala	4.7	5.5	5.2	4.9	4.6	4.3	4.0	3.4	2.7	2.0
Roberts	6.9	6.0	5.1	4.2	3.4	2.5	1.6	0.7	0.0	0.0
Maverick	2.5	3.0	3.6	4.2	4.8	4.5	4.0	3.6	3.1	2.6
Cooke	11.9	9.3	6.7	4.1	1.5	0.0	0.0	0.0	0.0	0.0
Ward	2.7	3.2	4.2	4.1	4.0	3.6	3.2	2.7	2.3	1.9
Austin	0.0	1.2	2.5	3.7	3.4	3.0	2.6	2.2	1.9	1.5
Reeves	1.4	1.8	2.7	3.7	3.9	3.6	3.3	3.0	2.6	2.3

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Glasscock	3.1	4.1	3.9	3.6	3.1	2.6	2.1	1.5	1.0	0.7
Tyler	1.9	2.6	3.2	3.2	2.8	2.4	2.0	1.6	1.1	0.7
Hood	1.4	2.0	2.6	3.2	2.9	2.6	2.2	1.9	1.6	1.3
Garza	1.5	2.0	2.5	2.9	2.7	2.4	2.1	1.8	1.5	1.2
Andrews	2.3	3.0	2.9	2.7	2.6	2.3	2.0	1.7	1.4	1.1
Crane	1.3	1.7	2.1	2.6	3.1	2.8	2.5	2.2	1.9	1.7
Erath	0.9	1.4	1.9	2.4	2.2	2.0	1.8	1.6	1.4	1.2
Wise	3.6	3.2	2.8	2.4	2.0	1.6	1.2	0.8	0.4	0.0
Upshur	0.2	0.9	1.7	2.4	2.9	2.6	2.3	2.1	1.8	1.5
Mitchell	1.2	1.6	2.0	2.4	2.1	1.9	1.7	1.4	1.2	0.9
Ector	1.5	2.0	2.1	2.3	2.2	1.9	1.7	1.4	1.2	1.0
Culberson	0.3	0.4	1.3	2.2	2.9	2.6	2.4	2.1	1.9	1.6
Lipscomb	1.7	3.0	2.6	2.1	1.7	1.3	0.8	0.4	0.0	0.0
Angelina	0.4	0.9	1.5	2.1	2.2	2.0	1.8	1.6	1.4	1.2
Houston	2.1	2.7	2.4	2.1	1.8	1.5	1.2	0.9	0.6	0.3
Frio	1.8	1.8	1.9	1.9	1.8	1.8	1.7	1.5	1.2	0.9
Newton	1.8	2.3	2.1	1.8	1.6	1.3	1.0	0.8	0.5	0.3
Kleberg	1.0	1.4	1.7	1.7	1.5	1.3	1.1	0.8	0.6	0.4
Brooks	1.0	1.3	1.7	1.7	1.5	1.2	1.0	0.8	0.6	0.4
Brazos	0.4	0.9	1.2	1.5	1.4	1.2	1.0	0.8	0.7	0.5
Comanche	0.4	0.7	1.0	1.4	1.2	1.1	1.0	0.8	0.7	0.5
Ochiltree	0.6	1.1	1.5	1.2	1.0	0.7	0.5	0.2	0.0	0.0

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Palo Pinto	0.3	0.6	0.9	1.2	1.1	1.0	0.8	0.7	0.6	0.5
Limestone	0.9	1.0	1.1	1.2	1.1	1.0	0.8	0.7	0.6	0.4
Duval	0.7	0.9	1.1	1.1	1.0	0.8	0.7	0.5	0.4	0.3
Stephens	0.1	0.4	0.8	1.1	1.0	0.9	0.8	0.6	0.5	0.4
Dawson	0.5	0.8	1.0	1.1	1.1	1.0	0.8	0.6	0.5	0.3
Scurry	0.0	0.6	0.8	1.0	1.2	1.1	0.9	0.8	0.7	0.5
Bee	0.8	1.1	1.1	1.0	0.9	0.7	0.6	0.4	0.3	0.1
Val Verde	0.0	0.5	0.8	0.9	1.1	1.0	0.9	0.8	0.6	0.5
Colorado	<0.1	0.3	0.6	0.9	0.8	0.7	0.6	0.5	0.4	0.4
Tarrant	2.1	1.7	1.3	0.9	0.4	0.0	0.0	0.0	0.0	0.0
Zapata	0.5	0.7	0.8	0.8	0.7	0.6	0.5	0.4	0.3	0.2
Ellis	0.3	0.5	0.6	0.8	0.7	0.6	0.6	0.5	0.4	0.3
Jim Wells	0.4	0.6	0.7	0.7	0.6	0.5	0.4	0.4	0.3	0.2
Lynn	0.0	0.4	0.6	0.7	0.8	0.8	0.7	0.6	0.5	0.4
Henderson	0.1	0.3	0.5	0.7	0.8	0.7	0.6	0.5	0.4	0.4
Hansford	0.0	0.4	0.8	0.7	0.5	0.4	0.3	0.2	0.1	0
Gaines	0.2	0.3	0.5	0.5	0.5	0.4	0.4	0.3	0.2	0.2
Gregg	0.1	0.2	0.3	0.4	0.4	0.4	0.4	0.3	0.3	0.2
Refugio	0.2	0.3	0.4	0.4	0.3	0.3	0.2	0.2	0.1	0.1
Caldwell	0.4	0.5	0.4	0.4	0.3	0.3	0.2	0.2	0.1	0.1
Pecos	0.1	0.1	0.2	0.4	0.5	0.4	0.4	0.3	0.3	0.2
Anderson	0.1	0.2	0.3	0.4	0.4	0.4	0.4	0.3	0.3	0.2

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Young	0.0	0.1	0.2	0.4	0.3	0.3	0.3	0.2	0.2	0.1
San Patricio	0.2	0.3	0.4	0.4	0.3	0.3	0.2	0.2	0.1	0.1
Smith	0.1	0.1	0.2	0.3	0.4	0.3	0.3	0.3	0.2	0.2
Cherokee	0.1	0.2	0.2	0.3	0.4	0.3	0.3	0.2	0.2	0.2
McLennan	0.1	0.1	0.2	0.3	0.3	0.2	0.2	0.2	0.2	0.1
Terry	0.0	0.2	0.2	0.3	0.3	0.3	0.3	0.2	0.2	0.2
Starr	0.2	0.2	0.3	0.3	0.2	0.2	0.2	0.1	0.1	0.1
Cochran	0.1	0.2	0.2	0.2	0.3	0.2	0.2	0.2	0.2	0.1
Jasper	0.2	0.3	0.2	0.2	0.2	0.1	0.1	0.1	0.1	<0.1
Dallas	0.2	0.3	0.2	0.2	0.1	0.1	<0.1	0.0	0.0	0.0
Robertson	0.1	0.2	0.2	0.2	0.2	0.1	0.1	0.1	0.1	0.1
Grimes	<0.1	0.1	0.1	0.2	0.1	0.1	0.1	0.1	0.1	0.1
Yoakum	0.1	0.1	0.2	0.2	0.1	0.1	0.1	0.1	0.1	0.1
Freestone	0.1	0.1	0.1	0.2	0.2	0.1	0.1	0.1	0.1	0.1
Cass	<0.1	0.1	0.1	0.2	0.2	0.2	0.1	0.1	0.1	0.1
Hutchinson	0.0	0.1	0.2	0.1	0.1	0.1	0.1	<0.1	<0.1	0.0
Rusk	<0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	<0.1
Willacy	<0.1	0.1	0.1	0.1	0.1	0.1	0.1	<0.1	<0.1	<0.1
Victoria	<0.1	0.1	0.1	0.1	0.1	0.1	<0.1	<0.1	<0.1	<0.1
Sherman	0.0	0.0	<0.1	0.1	0.1	0.1	<0.1	<0.1	<0.1	<0.1
Calhoun	<0.1	0.1	0.1	0.1	0.1	0.1	<0.1	<0.1	<0.1	<0.1
Lubbock	0.0	0.0	<0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Jackson	<0.1	<0.1	0.1	0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Matagorda	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Polk	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Wharton	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Nueces	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Hidalgo	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Cameron	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Somervell	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Goliad	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Brazoria	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Fort Bend	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
Aransas	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Armstrong	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bailey	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bandera	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bastrop	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Baylor	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bell	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bexar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Blanco	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Bowie	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Brewster	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Briscoe	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Brown	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Burnet	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Callahan	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Camp	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Carson	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Castro	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Chambers	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Childress	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Coke	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Coleman	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Collin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Collingsworth	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Comal	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Concho	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Cottle	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Crosby	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Dallam	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Deaf Smith	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Delta	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Denton	1.7	1.1	0.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Dickens	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Donley	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Edwards	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
El Paso	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Falls	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Fannin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Fisher	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Floyd	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Foard	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Franklin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Galveston	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Gillespie	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Gray	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Grayson	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Guadalupe	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hale	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hardeman	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hardin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Harris	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hartley	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Haskell	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hays	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Hockley	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hopkins	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hudspeth	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hunt	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Jeff Davis	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Jefferson	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Jones	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kaufman	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kendall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kent	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kerr	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kimble	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
King	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Kinney	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Knox	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lamar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lamb	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lampasas	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Liberty	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Llano	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
McCulloch	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mason	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
Medina	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Menard	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Milam	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mills	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Montgomery	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Moore	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Morris	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Motley	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Navarro	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Nolan	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Oldham	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Orange	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Parmer	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Potter	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Presidio	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Rains	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Randall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Real	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Red River	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Rockwall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Runnels	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
San Jacinto	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

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Texas county	Projected hydraulic fracturing water use as a percentage of 2010 total water use <sup>a,b</sup>									
	2015	2020	2025	2030	2035	2040	2045	2050	2055	2060
San Saba	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Stonewall	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Swisher	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Taylor	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Throckmorton	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Titus	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Tom Green	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Travis	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Trinity	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Uvalde	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Van Zandt	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Walker	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Waller	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Wichita	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Wilbarger	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Williamson	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Wood	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

<sup>a</sup> Total water use data accessed from the USGS website (<http://water.usgs.gov/watuse/data/2010/>) on April 21, 2015. Data from [Nicot et al. \(2012\)](#) transcribed.

<sup>b</sup> Percentages calculated by dividing projected hydraulic fracturing water use volumes from [Nicot et al. \(2012\)](#) by 2010 total water use from the USGS and multiplying by 100. Percentages less than 0.1 were not rounded and simply noted as “<0.1”, but where the percentage was actually zero because there was no projected hydraulic fracturing water use we noted that as “0.0”.

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## Appendix C

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# Chemical Mixing Supplemental Tables and Information

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## Appendix C. Chemical Mixing Supplemental Tables and Information

### C.1. Supplemental Tables and Information

**Table C-1. Chemicals reported to FracFocus in 10% or more of disclosures for gas-producing wells, with the number of disclosures where chemical is reported, percentage of disclosures, and the median maximum concentration (% by mass) of that chemical in hydraulic fracturing fluid.**

Chemicals ranked by frequency of occurrence ([U.S. EPA, 2015c](#)).

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Hydrochloric acid	7647-01-0	12,351	72.8%	15%
Methanol	67-56-1	12,269	72.3%	30%
Distillates, petroleum, hydrotreated light	64742-47-8	11,897	70.1%	30%
Isopropanol	67-63-0	8,008	47.2%	30%
Water	7732-18-5	7,998	47.1%	63%
Ethanol	64-17-5	6,325	37.3%	5%
Propargyl alcohol	107-19-7	5,811	34.2%	10%
Glutaraldehyde	111-30-8	5,635	33.2%	30%
Ethylene glycol	107-21-1	5,493	32.4%	35%
Citric acid	77-92-9	4,832	28.5%	60%
Sodium hydroxide	1310-73-2	4,656	27.4%	5%
Peroxydisulfuric acid, diammonium salt	7727-54-0	4,618	27.2%	100%
Quartz	14808-60-7	3,758	22.1%	10%
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	3,668	21.6%	100%
Sodium chloride	7647-14-5	3,608	21.3%	30%
Guar gum	9000-30-0	3,586	21.1%	60%
Acetic acid	64-19-7	3,563	21.0%	50%
2-Butoxyethanol	111-76-2	3,325	19.6%	10%
Naphthalene	91-20-3	3,294	19.4%	5%
Solvent naphtha, petroleum, heavy arom.	64742-94-5	3,287	19.4%	30%
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1	3,259	19.2%	7%
Potassium hydroxide	1310-58-3	2,843	16.8%	15%
Ammonium chloride	12125-02-9	2,483	14.6%	10%
Choline chloride	67-48-1	2,477	14.6%	75%

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Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0	2,455	14.5%	5%
Sodium chlorite	7758-19-2	2,372	14.0%	10%
1,2,4-Trimethylbenzene	95-63-6	2,229	13.1%	1%
Carbonic acid, dipotassium salt	584-08-7	2,154	12.7%	60%
Methenamine	100-97-0	2,134	12.6%	1%
Formic acid	64-18-6	2,118	12.5%	60%
Didecyl dimethyl ammonium chloride	7173-51-5	2,063	12.2%	10%
N,N-Dimethylformamide	68-12-2	1,892	11.2%	13%
Phenolic resin	9003-35-4	1,852	10.9%	5%
Thiourea polymer	68527-49-1	1,702	10.0%	30%
Polyethylene glycol	25322-68-3	1,696	10.0%	60%

Note: Analysis considered 17,035 disclosures and 291,363 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (1,587) or other, query-specific criteria were excluded from analysis.

**Table C-2. Chemicals reported to FracFocus in 10% or more of disclosures for oil-producing wells, with the number of disclosures where chemical is reported, percentage of disclosures, and the median maximum concentration (% by mass) of that chemical in hydraulic fracturing fluid.**

Chemicals ranked by frequency of occurrence ([U.S. EPA, 2015c](#)).

Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Methanol	67-56-1	12,484	71.8%	30%
Distillates, petroleum, hydrotreated light	64742-47-8	10,566	60.8%	40%
Peroxydisulfuric acid, diammonium salt	7727-54-0	10,350	59.6%	100%
Ethylene glycol	107-21-1	10,307	59.3%	30%
Hydrochloric acid	7647-01-0	10,029	57.7%	15%
Guar gum	9000-30-0	9,110	52.4%	50%
Sodium hydroxide	1310-73-2	8,609	49.5%	10%
Quartz	14808-60-7	8,577	49.4%	2%
Water	7732-18-5	8,538	49.1%	67%
Isopropanol	67-63-0	8,031	46.2%	15%
Potassium hydroxide	1310-58-3	7,206	41.5%	15%
Glutaraldehyde	111-30-8	5,927	34.1%	15%
Propargyl alcohol	107-19-7	5,599	32.2%	5%
Acetic acid	64-19-7	4,623	26.6%	30%
2-Butoxyethanol	111-76-2	4,022	23.1%	10%
Solvent naphtha, petroleum, heavy arom.	64742-94-5	3,821	22.0%	5%
Sodium chloride	7647-14-5	3,692	21.2%	25%
Ethanol	64-17-5	3,536	20.3%	45%
Citric acid	77-92-9	3,310	19.0%	60%
Phenolic resin	9003-35-4	3,109	17.9%	5%
Naphthalene	91-20-3	3,060	17.6%	5%
Nonyl phenol ethoxylate	9016-45-9	2,829	16.3%	20%
Diatomaceous earth, calcined	91053-39-3	2,655	15.3%	100%
Methenamine	100-97-0	2,559	14.7%	1%
Tetramethylammonium chloride	75-57-0	2,428	14.0%	1%
Carbonic acid, dipotassium salt	584-08-7	2,402	13.8%	60%
Ethoxylated propoxylated C12-14 alcohols	68439-51-0	2,342	13.5%	2%
Choline chloride	67-48-1	2,264	13.0%	75%
Boron sodium oxide	1330-43-4	2,228	12.8%	30%
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	2,130	12.3%	50%
1,2,4-Trimethylbenzene	95-63-6	2,118	12.2%	1%

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Chemical name	CASRN	Number of disclosures	Percentage of disclosures	Median maximum concentration in hydraulic fracturing fluid (% by mass)
Boric acid	10043-35-3	2,070	11.9%	25%
Polyethylene glycol	25322-68-3	2,025	11.7%	5%
2-Mercaptoethanol	60-24-2	2,012	11.6%	100%
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1,988	11.4%	98%
Formic acid	64-18-6	1,948	11.2%	60%
Sodium persulfate	7775-27-1	1,914	11.0%	100%
Phosphonic acid	13598-36-2	1,865	10.7%	1%
Sodium tetraborate decahydrate	1303-96-4	1,862	10.7%	30%
Potassium metaborate	13709-94-9	1,682	9.7%	60%
Ethylenediaminetetraacetic acid tetrasodium salt hydrate	64-02-8	1,676	9.6%	0%
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0	1,668	9.6%	5%

Note: Analysis considered 17,640 disclosures and 385,013 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (2,268) or other, query-specific criteria were excluded from analysis.

**Table C-3a. Top chemicals reported to FracFocus for each state and number (and percentage) of disclosures where a chemical is reported for that state, Alabama to Montana (U.S. EPA, 2015c).**

Source: (U.S. EPA, 2015c). The top 20 most frequent chemicals were identified for the 20 states that reported to FracFocus, resulting in a total of 93 chemicals. The chemicals were ranked by counting the number of states where that chemical was in the top 20; chemicals used most widely among the most states come first. For example, methanol is reported in 19 of 20 states, so methanol is ranked first.

Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Methanol	67-56-1	55 (100%)		1333 (99.7%)	228 (39.0%)	2883 (63.3%)	77 (79.4%)	596 (59.2%)	13 (92.9%)	3 (75%)	121 (62.7%)
Distillates, petroleum, hydrotreated light	64742-47-8		9 (45%)	743 (55.6%)	322 (55.0%)	3358 (73.7%)	87 (89.7%)	844 (83.9%)	14 (100%)	4 (100%)	115 (59.6%)
Ethylene glycol	107-21-1	55 (100%)	20 (100%)	291 (21.8%)	350 (59.8%)		61 (62.9%)	341 (33.9%)	10 (71.4%)	3 (75%)	95 (49.2%)
Isopropanol	67-63-0	55 (100%)	13 (65%)	586 (43.9%)		2586 (56.8%)	24 (24.7%)	515 (51.2%)	11 (78.6%)		123 (63.7%)
Quartz	14808-60-7		20 (100%)		519 (88.7%)	1048 (23.0%)	22 (22.7%)	377 (37.5%)		2 (50%)	124 (64.2%)
Sodium hydroxide	1310-73-2		20 (100%)	285 (21.3%)	403 (68.9%)	996 (21.9%)	27 (27.8%)	535 (53.2%)		2 (50%)	105 (54.4%)
Ethanol	64-17-5			603 (45.1%)		2258 (49.6%)	78 (80.4%)	420 (41.7%)		4 (100%)	
Guar gum	9000-30-0		10 (50%)		545 (93.2%)			494 (49.1%)		2 (50%)	83 (43.0%)
Hydrochloric acid	7647-01-0	55 (100%)		1330 (99.5%)		2408 (52.9%)	82 (84.5%)	569 (56.6%)			45 (23.3%)
Peroxydisulfuric acid, diammonium salt	7727-54-0		10 (50%)		484 (82.7%)		21 (21.6%)	273 (27.2%)	8 (57.1%)		119 (61.7%)

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Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Propargyl alcohol	107-19-7			813 (60.8%)			69 (71.1%)	299 (29.7%)	5 (35.7%)		
Glutaraldehyde	111-30-8			737 (55.1%)			73 (75.3%)	364 (36.3%)		2 (50%)	
Naphthalene	91-20-3	55 (100%)				1363 (29.9%)	41 (42.3%)	293 (29.2%)	12 (85.7%)		95 (49.2%)
2-Butoxyethanol	111-76-2	55 (100%)	20 (100%)						11 (78.6%)		
Citric acid	77-92-9						45 (46.4%)				
Saline	7647-14-5					1574 (34.5%)		408 (40.6%)		2 (50%)	
Solvent naphtha, petroleum, heavy arom.	64742-94-5					1507 (33.1%)	42 (43.3%)				135 (70.0%)
Quaternary ammonium compounds, benzyl-C12- 16-alkyldimethyl, chlorides	68424-85-1			375 (28.0%)			52 (53.6%)			2 (50%)	
2,2-Dibromo-3- nitrilopropionamide	10222-01-2	55 (100%)				2215 (48.6%)			10 (71.4%)		70 (36.3%)
Potassium hydroxide	1310-58-3							340 (33.8%)		4 (100%)	115 (59.6%)
Choline chloride	67-48-1					1235 (27.1%)					
Polyethylene glycol	25322-68-3	55 (100%)							7 (50%)		69 (35.8%)
1,2,4-Trimethylbenzene	95-63-6					1211 (26.63%)	39 (40.2%)				

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Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Ammonium chloride	12125-02-9			277 (20.7%)		1280 (28.0%)					
Diatomaceous earth, calcined	91053-39-3		20 (100%)		417 (71.3%)						
Didecyl dimethyl ammonium chloride	7173-51-5			317 (23.7%)						2 (50%)	
Sodium chlorite	7758-19-2							352 (35.0%)		4 (100%)	
Sodium erythorbate	6381-77-7			435 (32.5%)			29 (29.9%)				
N,N-Dimethylformamide	68-12-2										
Nonyl phenol ethoxylate	9016-45-9										
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0				1150 (25.2%)	39 (40.2%)					
Sodium persulfate	7775-27-1									4 (100%)	
Tetramethylammonium chloride	75-57-0										85 (44.0%)
1,2-Propylene glycol	57-55-6								10 (71.4%)		
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4		20 (100%)		389 (66.5%)						
Acetic acid	64-19-7					959 (21.0%)		284 (28.2%)			
Ammonium acetate	631-61-8									2 (50%)	

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Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Boric acid	10043-35-3		3 (15%)								
Carbonic acid, dipotassium salt	584-08-7					1159 (25.4%)					
Cristobalite	14464-46-1		20 (100%)		389 (66.5%)						
Formic acid	64-18-6	55 (100%)						293 (29.1%)			
Hemicellulase enzyme	9012-54-8										
Hemicellulase enzyme concentrate	9025-56-3				395 (67.5%)						
Iron(II) sulfate heptahydrate	7782-63-0								7 (50%)		
Magnesium chloride	7786-30-3		20 (100%)		389 (66.5%)						
Magnesium nitrate	10377-60-3		20 (100%)		389 (66.5%)						
Phenolic resin	9003-35-4										
Sodium hypochlorite	7681-52-9					1046 (23.0%)					
Sodium tetraborate decahydrate	1303-96-4		14 (70%)								
Solvent naphtha, petroleum, heavy aliph.	64742-96-7								7 (50%)	2 (50%)	
1-Butoxy-2-propanol	5131-66-8				315 (53.8%)						

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Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
1-Propanol	71-23-8					1232 (27.0%)					
1,2-Ethanediaminium, N, N'-bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'bis(2-hydroxyethyl)-N,N'-dimethyl-,tetrachloride	138879-94-4			343 (58.6%)							
2-bromo-3-nitrilopropionamide	1113-55-9										
2-Ethylhexanol	104-76-7										83 (43.0052%)
2-Methyl-3(2H)-isothiazolone	2682-20-4		20 (100%)		389 (66.5%)						
2-Propenoic acid, polymer with 2-propenamide	9003-06-9										
Alkenes, C>10 .alpha.-	64743-02-8			241 (18.0%)							
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated	119345-03-8										50 (25.9%)
Benzenesulfonic acid, dodecyl-, compd. with N1-(2-aminoethyl)-1,2-ethanediamine (1:?)	40139-72-8										48 (24.9%)
Benzyl dimethyldodecyl ammonium chloride	139-07-1			268 (20.0%)							

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Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Benzylhexadecyldimethylammonium chloride	122-18-9			268 (20.0%)							
Boron sodium oxide	1330-43-4				361 (61.7%)						
C10-C16 ethoxylated alcohol	68002-97-1		3 (15%)								
Calcium chloride	10043-52-4		20 (100%)								
Carbon dioxide	124-38-9								7 (50%)		
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	55 (100%)									
Diethylene glycol	111-46-6										
Diethylene glycol monobutyl ether	112-34-5								7 (50%)		
Diethylenetriamine	111-40-0										55 (28.5%)
Distillates, petroleum, hydrotreated light paraffinic	64742-55-8				314 (53.7%)						
Distillates, petroleum, hydrotreated middle	64742-46-7		3 (15%)								
Ethoxylated C12-16 alcohols	68551-12-2										
Ethoxylated C14-15 alcohols	68951-67-7			241 (18.0%)							
Formic acid, potassium salt	590-29-4										

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Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Glycerin, natural	56-81-5								7 (50%)		
Isotridecanol, ethoxylated	9043-30-5				312 (53.3%)						
Methenamine	100-97-0							298 (29.6%)			
Naphtha, petroleum, hydrotreated heavy	64742-48-9										
Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[[(9Z)-9-octadecenylimino]di-2,1-ethanediyl]bis[.omega.-hydroxy-	26635-93-8								9 (64.3%)		
Potassium chloride	7447-40-7								7 (50%)		
Sodium bromate	7789-38-0								7 (50%)		
Sodium perborate tetrahydrate	10486-00-7										
Sulfamic acid	5329-14-6									2 (50%)	
Terpenes and Terpenoids, sweet orange-oil	68647-72-3									2 (50%)	
Tetradecyl dimethyl benzyl ammonium chloride	139-08-2			268 (20.0%)							
Tetrakis(hydroxymethyl)p hosphonium sulfate	55566-30-8										

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Chemical name	CASRN	Alabama	Alaska	Arkansas	California	Colorado	Kansas	Louisiana	Michigan	Mississippi	Montana
Thiourea polymer	68527-49-1			384 (28.7%)							
Tri-n-butyl tetradecyl phosphonium chloride	81741-28-8										
Trisodium phosphate	7601-54-9						19 (19.6%)				

Note for Table C-3a and C-3b: Analysis considered 34,675 disclosures and 676,376 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (3,855) or other, query-specific criteria were excluded from analysis.

**Table C-3b. Top chemicals reported to FracFocus for each state and number (and percentage) of disclosures where a chemical is reported for that state, New Mexico to Wyoming (U.S. EPA, 2015c).**

Source: ([U.S. EPA, 2015c](#)). The top 20 most frequent chemicals were identified for the 20 states that reported to FracFocus, resulting in a total of 93 chemicals. The chemicals were ranked by counting the number of states where that chemical was in the top 20; chemicals used most widely among the most states come first. For example, methanol is reported in 19 of 20 states, so methanol is ranked first.

Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Methanol	67-56-1	1012 (90.8%)	1059 (53.3%)	76 (52.1%)	1270 (70.3%)	1633 (68.6%)	12664 (78.5%)	984 (78.5%)	48 (60.8%)	153 (64.0%)	460 (38.4%)
Distillates, petroleum, hydrotreated light	64742-47-8	699 (62.7%)	943 (47.5%)	122 (83.6%)	1270 (70.3%)	1434 (60.2%)	10677 (66.1%)	934 (74.5%)		196 (82.0%)	612 (51.1%)
Ethylene glycol	107-21-1	503 (45.1%)	724 (36.4%)	83 (56.8%)	843 (46.7%)	807 (33.9%)	9591 (59.4%)	1065 (85.0%)	22 (27.8%)	141 (59.0%)	
Isopropanol	67-63-0	695 (62.3%)	739 (37.2%)	71 (48.6%)	764 (42.28%)	735 (30.9%)	7731 (47.9%)	661 (52.8%)	43 (54.4%)	74 (31.0%)	516 (43.1%)

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Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Quartz	14808-60-7	762 (68.3%)	920 (46.3%)	66 (45.2%)	491 (27.2%)		6869 (42.6%)	503 (40.1%)		53 (22.2%)	356 (29.7%)
Sodium hydroxide	1310-73-2	329 (29.5%)	1028 (51.7%)		490 (27.1%)	406 (17.0%)	7371 (45.7%)	466 (37.2%)			688 (57.4%)
Ethanol	64-17-5	529 (47.4%)	545 (27.4%)	87 (59.6%)	838 (46.4%)	388 (16.3%)	3439 (21.3%)		50 (63.3%)	130 (54.3%)	298 (24.9%)
Guar gum	9000-30-0	702 (63.0%)	1094 (55.1%)	74 (50.7%)	457 (25.3%)	538 (22.6%)	6863 (42.5%)	538 (42.9%)		55 (23.0%)	823 (68.7%)
Hydrochloric acid	7647-01-0	880 (78.9%)		145 (99.3%)	1372 (75.9%)	2279 (95.7%)	11424 (70.8%)	1064 (84.9%)	68 (86.1%)	229 (95.8%)	
Peroxydisulfuric acid, diammonium salt	7727-54-0	836 (75.0%)	1089 (54.8%)	93 (63.7%)	713 (39.5%)		8666 (53.7%)	483 (38.5%)		128 (53.6%)	771 (64.4%)
Propargyl alcohol	107-19-7	760 (68.2%)		72 (49.3%)	732 (40.5%)	1371 (57.6%)	6269 (38.8%)	456 (36.4%)	22 (27.8%)	138 (57.7%)	
Glutaraldehyde	111-30-8	632 (56.7%)		105 (71.9%)	989 (54.7%)	819 (34.4%)	6470 (40.1%)			169 (70.7%)	260 (21.7%)
Naphthalene	91-20-3		864 (43.5%)		448 (24.8%)			478 (38.1%)	7 (8.9%)		
2-Butoxyethanol	111-76-2	412 (37.0%)				498 (20.9%)	3898 (24.1%)	663 (52.9%)	70 (88.6%)	62 (25.9%)	
Citric acid	77-92-9	447 (40.1%)		96 (65.8%)	644 (35.6%)	701 (29.4%)	3820 (23.7%)	992 (79.2%)	63 (79.8%)	98 (41.0%)	
Saline	7647-14-5		491 (24.7%)				3462 (21.4%)		7 (8.9%)	53 (22.2%)	274 (22.9%)
Solvent naphtha, petroleum, heavy arom.	64742-94-5		981 (49.4%)		557 (30.8%)		2751 (17.0%)		7 (8.9%)		415 (34.6%)

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Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1			54 (37.0%)	597 (33.0%)	373 (15.7%)				53 (22.2%)	
2,2-Dibromo-3-nitrilopropionamide	10222-01-2					804 (33.8%)			22 (27.8%)		
Potassium hydroxide	1310-58-3		1176 (59.2%)	106 (72.6%)			6369 (39.5%)				
Choline chloride	67-48-1	384 (34.4%)		55 (37.7%)				649 (51.8%)	45 (57.0%)		
Polyethylene glycol	25322-68-3		567 (28.5%)			688 (28.9%)					
1,2,4-Trimethylbenzene	95-63-6		496 (25.0%)						7 (8.9%)		
Ammonium chloride	12125-02-9					732 (30.7%)				50 (20.9%)	
Diatomaceous earth, calcined	91053-39-3	419 (37.6%)						435 (34.7%)			
Didecyl dimethyl ammonium chloride	7173-51-5			46 (31.6%)						49 (20.5%)	
Sodium chlorite	7758-19-2		482 (24.3%)								271 (22.6%)
Sodium erythorbate	6381-77-7								10 (12.7%)	76 (31.8%)	
N,N-Dimethylformamide	68-12-2			68 (46.6%)	355 (19.6%)			410 (32.7%)			
Nonyl phenol ethoxylate	9016-45-9	333 (29.9%)						447 (35.7%)	25 (31.6%)		

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Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Poly(oxy-1,2-ethanediyl)-nonylphenyl-hydroxy (mixture)	127087-87-0								7 (8.9%)		
Sodium persulfate	7775-27-1					373 (15.7%)					308 (25.7%)
Tetramethylammonium chloride	75-57-0		579 (29.1%)								315 (26.3%)
1,2-Propylene glycol	57-55-6								22 (27.8%)		
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4										
Acetic acid	64-19-7										
Ammonium acetate	631-61-8										323 (27.0%)
Boric acid	10043-35-3			82 (56.2%)							
Carbonic acid, dipotassium salt	584-08-7		482 (24.2%)								
Cristobalite	14464-46-1										
Formic acid	64-18-6										
Hemicellulase enzyme	9012-54-8					367 (15.4%)			11 (13.9%)		
Hemicellulase enzyme concentrate	9025-56-3	331 (29.7%)									
Iron(II) sulfate heptahydrate	7782-63-0								22 (27.8%)		
Magnesium chloride	7786-30-3										

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Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Magnesium nitrate	10377-60-3										
Phenolic resin	9003-35-4	419 (37.6%)					2903 (18.0%)				
Sodium hypochlorite	7681-52-9										282 (23.5%)
Sodium tetraborate decahydrate	1303-96-4										265 (22.1%)
Solvent naphtha, petroleum, heavy aliph.	64742-96-7										
1-Butoxy-2-propanol	5131-66-8										
1-Propanol	71-23-8										
1,2-Ethanediaminium, N, N'-bis[2-[bis(2-hydroxy ethyl) methylammonio] ethyl]-N,N'bis(2-hydroxyethyl)-N,N'-dimethyl-, tetrachloride	138879-94-4										
2-Bromo-3-nitrilopropionamide	1113-55-9								11 (13.9%)		
2-Ethylhexanol	104-76-7										
2-Methyl-3(2H)-isothiazolone	2682-20-4										
2-Propenoic acid, polymer with 2-propenamide	9003-06-9							486 (38.8%)			
Alkenes, C>10 .alpha.-	64743-02-8										

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Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Benzene, 1,1'-oxybis-, tetrapropylene derivs., sulfonated	119345-03-8										
Benzenesulfonic acid, dodecyl-, compd. with N1-(2-aminoethyl)-1,2-ethanediamine (1:?)	40139-72-8										
Benzyltrimethylammonium chloride	139-07-1										
Benzylhexadecyltrimethylammonium chloride	122-18-9										
Boron sodium oxide	1330-43-4										
C10-C16 ethoxylated alcohol	68002-97-1										
Calcium chloride	10043-52-4										
Carbon dioxide	124-38-9										
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2										
Diethylene glycol	111-46-6			45 (30.8%)							
Diethylene glycol monobutyl ether	112-34-5										
Diethylenetriamine	111-40-0										
Distillates, petroleum, hydrotreated light paraffinic	64742-55-8										

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Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Distillates, petroleum, hydrotreated middle	64742-46-7										
Ethoxylated C12-16 alcohols	68551-12-2									57 (23.8%)	
Ethoxylated C14-15 alcohols	68951-67-7										
Formic acid, potassium salt	590-29-4										361 (30.1%)
Glycerin, natural	56-81-5										
Isotridecanol, ethoxylated	9043-30-5										
Methenamine	100-97-0										
Naphtha, petroleum, hydrotreated heavy	64742-48-9										384 (32.1%)
Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[[(9Z)-9-octadecenylimino]di-2,1-ethanediyl]bis[.omega.-hydroxy-	26635-93-8										
Potassium chloride	7447-40-7										
Sodium bromate	7789-38-0										
Sodium perborate tetrahydrate	10486-00-7				351 (19.4%)						
Sulfamic acid	5329-14-6										
Terpenes and terpenoids, sweet orange-oil	68647-72-3										

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Chemical name	CASRN	New Mexico	North Dakota	Ohio	Oklahoma	Pennsylvania	Texas	Utah	Virginia	West Virginia	Wyoming
Tetradecyl dimethyl benzyl ammonium chloride	139-08-2										
Tetrakis(hydroxymethyl)p hosphonium sulfate	55566-30-8							945 (75.4%)			
Thiourea polymer	68527-49-1										
Tri-n-butyl tetradecyl phosphonium chloride	81741-28-8					350 (14.7%)					
Trisodium phosphate	7601-54-9										

Note for Table C-3a and C-3b: Analysis considered 34,675 disclosures and 676,376 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (3,855) or other, query-specific criteria were excluded from analysis.

**Table C-4. Estimated mean, median, 5<sup>th</sup> percentile, and 95<sup>th</sup> percentile volumes in gallons for chemicals reported to FracFocus in 100 or more disclosures, where density information was available.**

Chemicals are listed in alphabetical order. Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7.

Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	2,702	406	0	19,741
1-Butoxy-2-propanol	5131-66-8	167	21	5	654
1-Decanol	112-30-1	28	4	0	33
1-Octanol	111-87-5	5	4	0	10
1-Propanol	71-23-8	128	55	6	367
1,2-Propylene glycol	57-55-6	13,105	72	4	61,071
1,2,4-Trimethylbenzene	95-63-6	38	6	0	43
2-Butoxyethanol	111-76-2	385	26	0	1,811
2-Ethylhexanol	104-76-7	100	11	0	292
2-Mercaptoethanol	60-24-2	1,175	445	0	4,194
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	183	5	0	341
Acetic acid	64-19-7	646	47	0	1,042
Acetic anhydride	108-24-7	239	50	3	722
Acrylamide	79-06-1	95	3	0	57
Adipic acid	124-04-9	153	0	0	109
Aluminum chloride	7446-70-0	2	0	0	0
Ammonia	7664-41-7	44	35	2	138
Ammonium acetate	631-61-8	839	117	0	1,384
Ammonium chloride	12125-02-9	440	48	3	458
Ammonium hydroxide	1336-21-6	7	2	0	14
Benzyl chloride	100-44-7	52	0	0	40
Carbonic acid, dipotassium salt	584-08-7	467	113	0	1,729
Chlorine dioxide	10049-04-4	31	11	0	28
Choline chloride	67-48-1	2,131	290	28	4,364
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	68	3	0	697

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Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
Citric acid	77-92-9	163	20	1	269
Dibromoacetonitrile	3252-43-5	22	13	1	45
Diethylene glycol	111-46-6	168	16	0	102
Diethylenetriamine	111-40-0	92	21	0	207
Dodecane	112-40-3	190	31	0	151
Ethanol	64-17-5	831	121	1	2,645
Ethanolamine	141-43-5	70	30	0	283
Ethyl acetate	141-78-6	0	0	0	0
Ethylene glycol	107-21-1	614	184	4	2,470
Ferric chloride	7705-08-0	0	0	0	0
Formalin	50-00-0	200	0	0	8
Formic acid	64-18-6	501	38	1	1,229
Fumaric acid	110-17-8	2	0	0	12
Glutaraldehyde	111-30-8	1,313	122	2	1,165
Glycerin, natural	56-81-5	413	109	10	911
Glycolic acid	79-14-1	38	10	4	94
Hydrochloric acid	7647-01-0	28,320	3,110	96	26,877
Isopropanol	67-63-0	2,095	55	0	1,264
Isopropylamine	75-31-0	83	121	0	172
Magnesium chloride	7786-30-3	14	0	0	2
Methanol	67-56-1	1,218	110	2	3,731
Methenamine	100-97-0	3,386	100	0	3,648
Methoxyacetic acid	625-45-6	36	4	2	115
N,N-Dimethylformamide	68-12-2	119	10	0	216
Naphthalene	91-20-3	72	12	0	204
Nitrogen, liquid	7727-37-9	41,841	26,610	3,091	108,200
Ozone	10028-15-6	15,844	15,473	8,785	26,063
Peracetic acid	79-21-0	300	268	50	663
Phosphonic acid	13598-36-2	1,201	0	0	3
Phosphoric acid Divosan X-Tend formulation	7664-38-2	13	4	0	15
Potassium acetate	127-08-2	204	1	0	974

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Name	CASRN	Volume (gallons)			
		Mean	Median	5th Percentile	95th Percentile
Propargyl alcohol	107-19-7	183	2	0	51
Saline	7647-14-5	876	85	0	1,544
Saturated sucrose	57-50-1	1	1	0	2
Silica, amorphous	7631-86-9	6,877	8	0	38,371
Sodium carbonate	497-19-8	228	16	0	1,319
Sodium formate	141-53-7	0	0	0	0
Sodium hydroxide	1310-73-2	551	38	0	1,327
Sulfur dioxide	7446-09-5	0	0	0	0
Sulfuric acid	7664-93-9	3	0	0	3
tert-Butyl hydroperoxide (70% solution in Water)	75-91-2	156	64	0	557
Tetramethylammonium chloride	75-57-0	970	483	2	3,508
Thioglycolic acid	68-11-1	55	7	2	229
Toluene	108-88-3	18	0	0	11
Tridecane	629-50-5	190	31	0	190
Triethanolamine	102-71-6	846	60	0	2,264
Triethyl phosphate	78-40-0	55	1	0	533
Triethylene glycol	112-27-6	5,198	116	28	945
Triisopropanolamine	122-20-3	46	4	1	330
Trimethyl borate	121-43-7	83	40	4	283
Undecane	1120-21-4	273	29	0	1,641

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

**Table C-5. Estimated mean, median, 5<sup>th</sup> percentile, and 95<sup>th</sup> percentile volumes in liters for chemicals reported to FracFocus in 100 or more disclosures, where density information was available.**

Chemicals are listed in alphabetical order. Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7.

Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	10,229	1,536	0	74,729
1-Butoxy-2-propanol	5131-66-8	631	80	18	2,475
1-Decanol	112-30-1	107	14	1	123
1-Octanol	111-87-5	21	14	1	39
1-Propanol	71-23-8	483	208	22	1,391
1,2-Propylene glycol	57-55-6	49,607	274	15	231,179
1,2,4-Trimethylbenzene	95-63-6	145	24	0	165
2-Butoxyethanol	111-76-2	1,459	98	0	6,856
2-Ethylhexanol	104-76-7	377	40	1	1,106
2-Mercaptoethanol	60-24-2	4,449	1,685	0	15,878
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	692	18	0	1,292
Acetic acid	64-19-7	2,446	176	0	3,945
Acetic anhydride	108-24-7	906	189	12	2,734
Acrylamide	79-06-1	361	10	0	216
Adipic acid	124-04-9	578	0	0	414
Aluminum chloride	7446-70-0	6	0	0	0
Ammonia	7664-41-7	166	134	7	523
Ammonium acetate	631-61-8	3,177	444	0	5,238
Ammonium chloride	12125-02-9	1,666	182	11	1,733
Ammonium hydroxide	1336-21-6	27	6	1	52
Benzyl chloride	100-44-7	196	1	0	151
Carbonic acid, dipotassium salt	584-08-7	1,769	429	0	6,544
Chlorine dioxide	10049-04-4	117	43	1	106
Choline chloride	67-48-1	8,068	1,096	107	16,521
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	258	12	0	2,638
Citric acid	77-92-9	618	77	5	1,019

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Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
Dibromoacetonitrile	3252-43-5	82	50	4	170
Diethylene glycol	111-46-6	636	61	1	384
Diethylenetriamine	111-40-0	347	80	0	785
Dodecane	112-40-3	719	117	0	572
Ethanol	64-17-5	3,144	458	6	10,011
Ethanolamine	141-43-5	264	112	0	1,070
Ethyl acetate	141-78-6	0	0	0	0
Ethylene glycol	107-21-1	2,324	697	14	9,349
Ferric chloride	7705-08-0	0	0	0	0
Formalin	50-00-0	756	2	0	31
Formic acid	64-18-6	1,896	144	2	4,653
Fumaric acid	110-17-8	9	0	0	46
Glutaraldehyde	111-30-8	4,972	462	6	4,409
Glycerin, natural	56-81-5	1,565	412	38	3,447
Glycolic acid	79-14-1	146	39	14	356
Hydrochloric acid	7647-01-0	107,204	11,772	362	101,741
Isopropanol	67-63-0	7,932	210	1	4,786
Isopropylamine	75-31-0	314	458	0	652
Magnesium chloride	7786-30-3	52	0	0	8
Methanol	67-56-1	4,609	416	6	14,125
Methenamine	100-97-0	12,817	378	0	13,810
Methoxyacetic acid	625-45-6	136	17	8	436
N,N-Dimethylformamide	68-12-2	449	38	2	819
Naphthalene	91-20-3	271	44	0	774
Nitrogen, liquid	7727-37-9	158,384	100,731	11,700	409,583
Ozone	10028-15-6	59,976	58,570	33,254	98,658
Peracetic acid	79-21-0	1,137	1,016	190	2,511
Phosphonic acid	13598-36-2	4,547	2	0	11
Phosphoric acid Divosan X-Tend formulation	7664-38-2	51	15	0	57
Potassium acetate	127-08-2	775	3	0	3,690
Propargyl alcohol	107-19-7	693	9	0	193

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Name	CASRN	Volume (L)			
		Mean	Median	5th Percentile	95th Percentile
Saline	7647-14-5	3,317	321	0	5,844
Saturated sucrose	57-50-1	5	2	0	6
Silica, amorphous	7631-86-9	26,031	32	0	145,251
Sodium carbonate	497-19-8	862	62	0	4,991
Sodium formate	141-53-7	1	1	0	1
Sodium hydroxide	1310-73-2	2,087	144	1	5,024
Sulfur dioxide	7446-09-5	2	0	0	0
Sulfuric acid	7664-93-9	10	0	0	12
tert-Butyl hydroperoxide (70% solution in Water)	75-91-2	591	242	0	2,109
Tetramethylammonium chloride	75-57-0	3,672	1,830	8	13,279
Thioglycolic acid	68-11-1	208	28	6	868
Toluene	108-88-3	69	0	0	41
Tridecane	629-50-5	721	118	0	721
Triethanolamine	102-71-6	3,203	228	0	8,570
Triethyl phosphate	78-40-0	209	6	0	2,019
Triethylene glycol	112-27-6	19,676	439	106	3,579
Triisopropanolamine	122-20-3	174	16	4	1,249
Trimethyl borate	121-43-7	314	152	16	1,072
Undecane	1120-21-4	1,035	111	0	6,212

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

**Table C-6. Calculated mean, median, 5<sup>th</sup> percentile, and 95<sup>th</sup> percentile chemical masses reported to FracFocus in 100 or more disclosures, where density information was available.**

Density information came from Reaxys® and other sources. All density sources are referenced in Table C-7. Number of disclosures reported for each chemical is also included.

Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	8,593	1,290	0	62,772	578
1-Butoxy-2-propanol	5131-66-8	555	71	16	2,178	773
1-Decanol	112-30-1	89	12	1	102	434
1-Octanol	111-87-5	17	12	1	32	434
1-Propanol	71-23-8	386	167	18	1,113	1,481
1,2-Propylene glycol	57-55-6	51,095	282	15	238,114	1,023
1,2,4-Trimethylbenzene	95-63-6	126	21	0	143	3,976
2-Butoxyethanol	111-76-2	1,313	88	0	6,170	6,778
2-Ethylhexanol	104-76-7	313	34	0	918	1,291
2-Mercaptoethanol	60-24-2	489	185	0	1,747	2,051
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1,660	44	0	3,102	4,927
Acetic acid	64-19-7	2,544	183	0	4,103	7,643
Acetic anhydride	108-24-7	969	203	12	2,925	1,377
Acrylamide	79-06-1	408	11	0	244	251
Adipic acid	124-04-9	785	0	0	564	233
Aluminum chloride	7446-70-0	15	0	0	0	122
Ammonia	7664-41-7	111	90	4	351	398
Ammonium acetate	631-61-8	3,718	520	0	6,129	1,504
Ammonium chloride	12125-02-9	2,530	277	16	2,633	3,288
Ammonium hydroxide	1336-21-6	48	11	2	94	1,173
Benzyl chloride	100-44-7	214	1	0	165	1,833
Carbonic acid, dipotassium salt	584-08-7	4,298	1,042	0	15,902	4,093
Chlorine dioxide	10049-04-4	321	117	3	291	331
Choline chloride	67-48-1	9,440	1,282	125	19,329	4,241
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	284	13	0	2,902	1,377

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Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
Citric acid	77-92-9	989	123	8	1,630	7,503
Dibromoacetonitrile	3252-43-5	193	118	11	403	272
Diethylene glycol	111-46-6	712	68	1	430	1,732
Diethylenetriamine	111-40-0	330	76	0	746	784
Dodecane	112-40-3	539	88	0	429	131
Ethanol	64-17-5	2,484	361	4	7,908	9,233
Ethanolamine	141-43-5	267	113	0	1,081	585
Ethyl acetate	141-78-6	0	0	0	0	110
Ethylene glycol	107-21-1	2,557	767	15	10,283	14,767
Ferric chloride	7705-08-0	0	0	0	0	118
Formalin	50-00-0	816	2	0	34	456
Formic acid	64-18-6	2,313	176	2	5,677	3,781
Fumaric acid	110-17-8	15	0	0	75	224
Glutaraldehyde	111-30-8	4,972	462	6	4,409	10,963
Glycerin, natural	56-81-5	1,972	519	47	4,343	1,829
Glycolic acid	79-14-1	217	58	21	530	595
Hydrochloric acid	7647-01-0	107,204	11,772	362	101,741	20,996
Isopropanol	67-63-0	6,187	163	1	3,733	15,058
Isopropylamine	75-31-0	213	311	0	444	255
Magnesium chloride	7786-30-3	120	1	0	18	1,113
Methanol	67-56-1	3,641	329	5	11,159	23,225
Methenamine	100-97-0	15,380	454	0	16,572	4,412
Methoxyacetic acid	625-45-6	161	20	9	514	584
N,N-Dimethylformamide	68-12-2	422	36	2	770	2,972
Naphthalene	91-20-3	220	35	0	627	5,945
Nitrogen, liquid	7727-37-9	129,875	82,599	9,594	335,858	713
Ozone	10028-15-6	129	126	71	212	209
Peracetic acid	79-21-0	1,251	1,117	209	2,762	221
Phosphonic acid	13598-36-2	7,730	3	0	18	2,216
Phosphoric acid Divosan X-Tend formulation	7664-38-2	48	14	0	54	315
Potassium acetate	127-08-2	1,216	5	0	5,793	325

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Name	CASRN	Mass (kg)				Disclosures
		Mean	Median	5th Percentile	95th Percentile	
Propargyl alcohol	107-19-7	658	9	0	183	10,771
Saline	7647-14-5	7,197	696	0	12,682	6,673
Saturated sucrose	57-50-1	6	2	0	7	125
Silica, amorphous	7631-86-9	57,267	71	0	319,553	2,423
Sodium carbonate	497-19-8	2,191	158	0	12,678	396
Sodium formate	141-53-7	2	1	1	2	204
Sodium hydroxide	1310-73-2	4,445	306	2	10,701	12,585
Sulfur dioxide	7446-09-5	2	0	0	0	224
Sulfuric acid	7664-93-9	18	0	0	22	402
tert-Butyl hydroperoxide (70% solution in water)	75-91-2	532	218	0	1,898	814
Tetramethylammonium chloride	75-57-0	4,296	2,141	10	15,537	3,162
Thioglycolic acid	68-11-1	277	37	8	1,155	156
Toluene	108-88-3	59	0	0	35	214
Tridecane	629-50-5	541	88	0	541	132
Triethanolamine	102-71-6	3,588	255	0	9,599	1,498
Triethyl phosphate	78-40-0	222	6	0	2,140	991
Triethylene glycol	112-27-6	22,038	491	119	4,008	528
Triisopropanolamine	122-20-3	177	17	4	1,274	251
Trimethyl borate	121-43-7	292	141	14	997	294
Undecane	1120-21-4	766	82	0	4,597	241

Note: Analysis considered 34,495 disclosures and 672,358 ingredient records that met selected quality assurance criteria, including: completely parsed; unique combination of fracture date and API well number; fracture date between January 1, 2011, and February 28, 2013; criteria for water volumes; valid CASRN; and valid concentrations. Disclosures that did not meet quality assurance criteria (4,035) or other, query-specific criteria were excluded from analysis.

**Table C-7. Associated chemical densities and references used to calculate chemical mass and estimate chemical volume.**

Name	CASRN	Density (g/mL)	Reference
(4R)-1-methyl-4-(prop-1-en-2-yl)cyclohexene	5989-27-5	0.84	<a href="#">Dejoye Tanzi et al. (2012)</a>
1-Butoxy-2-propanol	5131-66-8	0.88	<a href="#">Pal et al. (2013)</a>
1-Decanol	112-30-1	0.83	<a href="#">Faria et al. (2013)</a>
1-Octanol	111-87-5	0.82	<a href="#">Dubey and Kumar (2013)</a>
1-Propanol	71-23-8	0.8	<a href="#">Rani and Maken (2013)</a>
1,2-Propylene glycol	57-55-6	1.03	<a href="#">Moosavi et al. (2013)</a>
1,2,4-Trimethylbenzene	95-63-6	0.87	<a href="#">He et al. (2008)</a>
2-Butoxyethanol	111-76-2	0.9	<a href="#">Dhondge et al. (2010)</a>
2-Ethylhexanol	104-76-7	0.83	<a href="#">Laavi et al. (2012)</a>
2-Mercaptoethanol	60-24-2	0.11	<a href="#">Rawat et al. (1976)</a>
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	2.4	<a href="#">Fels (1900)</a>
Acetic acid	64-19-7	1.04	<a href="#">Chafer et al. (2010)</a>
Acetic anhydride	108-24-7	1.07	<a href="#">Radwan and Hanna (1976)</a>
Acrylamide	79-06-1	1.13	<a href="#">Carpenter and Davis (1957)</a>
Adipic acid	124-04-9	1.36	<a href="#">Thalladi et al. (2000)</a>
Aluminum chloride	7446-70-0	2.44	<a href="#">Sigma-Aldrich (2015a)</a>
Ammonia	7664-41-7	0.67	<a href="#">Harlow et al. (1997)</a>
Ammonium acetate	631-61-8	1.17	<a href="#">Biltz and Balz (1928)</a>
Ammonium chloride	12125-02-9	1.519	<a href="#">Haynes (2014)</a>
Ammonium hydroxide	1336-21-6	1.8	<a href="#">Xiao et al. (2013)</a>
Benzyl chloride	100-44-7	1.09	<a href="#">Sarkar et al. (2012)</a>
Carbonic acid, dipotassium salt	584-08-7	2.43	<a href="#">Sigma-Aldrich (2014b)</a>
Chlorine dioxide	10049-04-4	2.757	<a href="#">Haynes (2014)</a>
Choline chloride	67-48-1	1.17	<a href="#">Shanley and Collin (1961)</a>
Cinnamaldehyde (3-phenyl-2-propenal)	104-55-2	1.1	<a href="#">Masood et al. (1976)</a>
Citric acid	77-92-9	1.6	<a href="#">Bennett and Yuill (1935)</a>
Dibromoacetonitrile	3252-43-5	2.37	<a href="#">Wilt (1956)</a>
Diethylene glycol	111-46-6	1.12	<a href="#">Chasib (2013)</a>
Diethylenetriamine	111-40-0	0.95	<a href="#">Dubey and Kumar (2011)</a>
Dodecane	112-40-3	0.75	<a href="#">Baragi et al. (2013)</a>

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Name	CASRN	Density (g/mL)	Reference
Ethanol	64-17-5	0.79	<a href="#">Kiselev et al. (2012)</a>
Ethanolamine	141-43-5	1.01	<a href="#">Blanco et al. (2013)</a>
Ethyl acetate	141-78-6	0.89	<a href="#">Laavi et al. (2013)</a>
Ethylene glycol	107-21-1	1.1	<a href="#">Rodnikova et al. (2012)</a>
Ferric chloride	7705-08-0	2.9	<a href="#">Haynes (2014)</a>
Formalin	50-00-0	1.08	<a href="#">Alfa Aesar (2015)</a>
Formic acid	64-18-6	1.22	<a href="#">Casanova et al. (1981)</a>
Fumaric acid	110-17-8	1.64	<a href="#">Huffman and Fox (1938)</a>
Glutaraldehyde	111-30-8	1	<a href="#">Oka (1962)</a>
Glycerin, natural	56-81-5	1.26	<a href="#">Egorov et al. (2013)</a>
Glycolic acid	79-14-1	1.49	<a href="#">Pijper (1971)</a>
Hydrochloric acid	7647-01-0	1	<a href="#">Steinhauser et al. (1990)</a>
Isopropanol	67-63-0	0.78	<a href="#">Zhang et al. (2013)</a>
Isopropylamine	75-31-0	0.68	<a href="#">Sarkar and Roy (2009)</a>
Magnesium chloride	7786-30-3	2.32	<a href="#">Haynes (2014)</a>
Methanol	67-56-1	0.79	<a href="#">Kiselev et al. (2012)</a>
Methenamine	100-97-0	1.2	<a href="#">Mak (1965)</a>
Methoxyacetic acid	625-45-6	1.18	<a href="#">Haynes (2014)</a>
N,N-Dimethylformamide	68-12-2	0.94	<a href="#">Smirnov and Badelin (2013)</a>
Naphthalene	91-20-3	0.81	<a href="#">Dyshin et al. (2008)</a>
Nitrogen, liquid	7727-37-9	0.8	<a href="#">finemech (2012)</a>
Ozone	10028-15-6	0.002144	<a href="#">Haynes (2014)</a>
Peracetic acid	79-21-0	1.1	<a href="#">Sigma-Aldrich (2015b)</a>
Phosphonic acid	13598-36-2	1.7	<a href="#">Sigma-Aldrich (2014a)</a>
Phosphoric acid Divosan X-Tend formulation	7664-38-2	0.94	<a href="#">Fadeeva et al. (2004)</a>
Potassium acetate	127-08-2	1.57	<a href="#">Haynes (2014)</a>
Propargyl alcohol	107-19-7	0.95	<a href="#">Vijaya Kumar et al. (1996)</a>
Saline	7647-14-5	2.17	<a href="#">Sigma-Aldrich (2010)</a>
Saturated sucrose	57-50-1	1.13	<a href="#">Hagen and Kaatze (2004)</a>
Silica, amorphous	7631-86-9	2.2	<a href="#">Fujino et al. (2004)</a>
Sodium carbonate	497-19-8	2.54	<a href="#">Haynes (2014)</a>
Sodium formate	141-53-7	1.97	<a href="#">Fuess et al. (1982)</a>

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Name	CASRN	Density (g/mL)	Reference
Sodium hydroxide	1310-73-2	2.13	<a href="#">Haynes (2014)</a>
Sulfur dioxide	7446-09-5	1.3	<a href="#">Sigma-Aldrich (2015c)</a>
Sulfuric acid	7664-93-9	1.83	<a href="#">Sigma-Aldrich (2015d)</a>
tert-Butyl hydroperoxide (70% solution in water)	75-91-2	0.9	<a href="#">Sigma-Aldrich (2007)</a>
Tetramethylammonium chloride	75-57-0	1.17	<a href="#">Haynes (2014)</a>
Thioglycolic acid	68-11-1	1.33	<a href="#">Biilmann (1906)</a>
Toluene	108-88-3	0.86	<a href="#">Martinez-Reina et al. (2012)</a>
Tridecane	629-50-5	0.75	<a href="#">Zhang et al. (2011)</a>
Triethanolamine	102-71-6	1.12	<a href="#">Blanco et al. (2013)</a>
Triethyl phosphate	78-40-0	1.06	<a href="#">Krakowiak et al. (2001)</a>
Triethylene glycol	112-27-6	1.12	<a href="#">Afzal et al. (2009)</a>
Triisopropanolamine	122-20-3	1.02	<a href="#">IUPAC (2014)</a>
Trimethyl borate	121-43-7	0.93	<a href="#">Sigma-Aldrich (2015e)</a>
Undecane	1120-21-4	0.74	<a href="#">de Oliveira et al. (2011)</a>

**Table C-8. Selected physicochemical properties of chemicals reported as used in hydraulic fracturing fluids.**

Properties are provided for chemicals, where available from EPI Suite™ version 4.1 ([U.S. EPA, 2012a](#)).

Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm·m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
(13Z)-N,N-bis(2-hydroxyethyl)-N-methyldocos-13-en-1-aminium chloride	120086-58-0	4.38	--	0.3827	$3.32 \times 10^{-15}$	--	--
(2,3-Dihydroxypropyl)trimethyl ammonium chloride	34004-36-9	-5.8	--	$1.00 \times 10^6$	$9.84 \times 10^{-18}$	--	--
(E)-Crotonaldehyde	123-73-9	0.6	--	$4.15 \times 10^4$	$5.61 \times 10^{-5}$	$1.90 \times 10^{-5}$	$1.94 \times 10^{-5}$
[Nitrilotris(methylene)]tris-phosphonic acid pentasodium salt	2235-43-0	-5.45	-3.53	$1.00 \times 10^6$	$1.65 \times 10^{-34}$	--	--
1-(1-Naphthylmethyl)quinolinium chloride	65322-65-8	5.57	--	0.02454	$1.16 \times 10^{-7}$	--	--
1-(Alkyl* amino)-3-aminopropane *(42%C12, 26%C18, 15%C14, 8%C16, 5%C10, 4%C8)	68155-37-3	4.74	--	23.71	$6.81 \times 10^{-8}$	$2.39 \times 10^{-8}$	--
1-(Phenylmethyl)pyridinium Et Me derivatives, chlorides	68909-18-2	4.1	--	14.13	$1.78 \times 10^{-5}$	--	--

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm·m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
1,2,3-Trimethylbenzene	526-73-8	3.63	3.66	75.03	$7.24 \times 10^{-3}$	$6.58 \times 10^{-3}$	$4.36 \times 10^{-3}$
1,2,4-Trimethylbenzene	95-63-6	3.63	3.63	79.59	$7.24 \times 10^{-3}$	$6.58 \times 10^{-3}$	$6.16 \times 10^{-3}$
1,2-Benzisothiazolin-3-one	2634-33-5	0.64	--	$2.14 \times 10^4$	$6.92 \times 10^{-9}$	--	--
1,2-Dibromo-2,4-dicyanobutane	35691-65-7	1.63	--	424	$3.94 \times 10^{-10}$	--	--
1,2-Dimethylbenzene	95-47-6	3.09	3.12	224.1	$6.56 \times 10^{-3}$	$6.14 \times 10^{-3}$	$5.18 \times 10^{-3}$
1,2-Ethanediaminium, N,N'-bis[2-[bis(2-hydroxyethyl)methylammonio]ethyl]-N,N'-bis(2-hydroxyethyl)-N,N'-dimethyl-, tetrachloride	138879-94-4	-23.19	--	$1.00 \times 10^6$	$2.33 \times 10^{-35}$	--	--
1,2-Propylene glycol	57-55-6	-0.78	-0.92	$8.11 \times 10^5$	$1.74 \times 10^{-7}$	$1.31 \times 10^{-10}$	$1.29 \times 10^{-8}$
1,2-Propylene oxide	75-56-9	0.37	0.03	$1.29 \times 10^5$	$1.60 \times 10^{-4}$	$1.23 \times 10^{-4}$	$6.96 \times 10^{-5}$
1,3,5-Triazine	290-87-9	-0.2	0.12	$1.03 \times 10^5$	$1.21 \times 10^{-6}$	--	--
1,3,5-Triazine-1,3,5(2H,4H,6H)-triethanol	4719-04-4	-4.67	--	$1.00 \times 10^6$	$1.08 \times 10^{-11}$	--	--

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm-m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
1,3,5-Trimethylbenzene	108-67-8	3.63	3.42	120.3	$7.24 \times 10^{-3}$	$6.58 \times 10^{-3}$	$8.77 \times 10^{-3}$
1,3-Butadiene	106-99-0	2.03	1.99	792.3	$7.79 \times 10^{-2}$	$7.05 \times 10^{-2}$	$7.36 \times 10^{-2}$
1,3-Dichloropropene	542-75-6	2.29	2.04	1,994	$2.45 \times 10^{-2}$	$3.22 \times 10^{-3}$	$3.55 \times 10^{-3}$
1,4-Dioxane	123-91-1	-0.32	-0.27	$2.14 \times 10^5$	$5.91 \times 10^{-6}$	$1.12 \times 10^{-7}$	$4.80 \times 10^{-6}$
1,6-Hexanediamine	124-09-4	0.35	--	$5.34 \times 10^5$	$3.21 \times 10^{-9}$	$7.05 \times 10^{-10}$	--
1,6-Hexanediamine dihydrochloride	6055-52-3	0.35	--	$5.34 \times 10^5$	$3.21 \times 10^{-9}$	$7.05 \times 10^{-10}$	--
1-[2-(2-Methoxy-1-methylethoxy)-1-methylethoxy]-2-propanol	20324-33-8	-0.2	--	$1.96 \times 10^5$	$2.36 \times 10^{-11}$	$4.55 \times 10^{-13}$	--
1-Amino-2-propanol	78-96-6	-1.19	-0.96	$1.00 \times 10^6$	$4.88 \times 10^{-10}$	$2.34 \times 10^{-10}$	--
1-Benzylquinolinium chloride	15619-48-4	4.4	--	6.02	$1.19 \times 10^{-6}$	--	--
1-Butanol	71-36-3	0.84	0.88	$7.67 \times 10^4$	$9.99 \times 10^{-6}$	$9.74 \times 10^{-6}$	$8.81 \times 10^{-6}$
1-Butoxy-2-propanol	5131-66-8	0.98	--	$4.21 \times 10^4$	$1.30 \times 10^{-7}$	$4.88 \times 10^{-8}$	--

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm·m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
1-Decanol	112-30-1	3.79	4.57	28.21	$5.47 \times 10^{-5}$	$7.73 \times 10^{-5}$	$3.20 \times 10^{-5}$
1-Dodecyl-2-pyrrolidinone	2687-96-9	5.3	4.2	5.862	$7.12 \times 10^{-7}$	--	--
1-Eicosene	3452-07-1	10.03	--	$1.26 \times 10^{-5}$	$1.89 \times 10^1$	$6.74 \times 10^1$	--
1-Ethyl-2-methylbenzene	611-14-3	3.58	3.53	96.88	$8.71 \times 10^{-3}$	$9.52 \times 10^{-3}$	$5.53 \times 10^{-3}$
1-Hexadecene	629-73-2	8.06	--	0.001232	6.10	$1.69 \times 10^1$	--
1-Hexanol	111-27-3	1.82	2.03	6,885	$1.76 \times 10^{-5}$	$1.94 \times 10^{-5}$	$1.71 \times 10^{-5}$
1-Methoxy-2-propanol	107-98-2	-0.49	--	$1.00 \times 10^6$	$5.56 \times 10^{-8}$	$1.81 \times 10^{-8}$	$9.20 \times 10^{-7}$
1-Octadecanamine, acetate (1:1)	2190-04-7	7.71	--	0.04875	$9.36 \times 10^{-4}$	$2.18 \times 10^{-3}$	--
1-Octadecanamine, N,N-dimethyl-	124-28-7	8.39	--	0.008882	$4.51 \times 10^{-3}$	$3.88 \times 10^{-2}$	--
1-Octadecene	112-88-9	9.04	--	$1.256 \times 10^{-4}$	10.7	$3.38 \times 10^1$	--
1-Octanol	111-87-5	2.81	3	814	$3.10 \times 10^{-5}$	$3.88 \times 10^{-5}$	$2.45 \times 10^{-5}$
1-Pentanol	71-41-0	1.33	1.51	$2.09 \times 10^4$	$1.33 \times 10^{-5}$	$1.38 \times 10^{-5}$	$1.30 \times 10^{-5}$

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm-m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
1-Propanaminium, 3-chloro-2-hydroxy-N,N,N-trimethyl-, chloride	3327-22-8	-4.48	--	$1.00 \times 10^6$	$9.48 \times 10^{-17}$	--	--
1-Propanesulfonic acid	5284-66-2	-1.4	--	$1.00 \times 10^6$	$2.22 \times 10^{-8}$	--	--
1-Propanol	71-23-8	0.35	0.25	$2.72 \times 10^5$	$7.52 \times 10^{-6}$	$6.89 \times 10^{-6}$	$7.41 \times 10^{-6}$
1-Propene	115-07-1	1.68	1.77	1,162	$1.53 \times 10^{-1}$	$1.58 \times 10^{-1}$	$1.96 \times 10^{-1}$
1-tert-Butoxy-2-propanol	57018-52-7	0.87	--	$5.24 \times 10^4$	$1.30 \times 10^{-7}$	$5.23 \times 10^{-8}$	--
1-Tetradecene	1120-36-1	7.08	--	0.01191	3.46	8.48	--
1-Tridecanol	112-70-9	5.26	--	4.533	$1.28 \times 10^{-4}$	$2.18 \times 10^{-4}$	--
1-Undecanol	112-42-5	4.28	--	43.04	$7.26 \times 10^{-5}$	$1.09 \times 10^{-4}$	--
2-(2-Butoxyethoxy)ethanol	112-34-5	0.29	0.56	$7.19 \times 10^4$	$1.52 \times 10^{-9}$	$4.45 \times 10^{-11}$	$7.20 \times 10^{-9}$
2-(2-Ethoxyethoxy)ethanol	111-90-0	-0.69	-0.54	$8.28 \times 10^5$	$8.63 \times 10^{-10}$	$2.23 \times 10^{-11}$	$2.23 \times 10^{-8}$
2-(2-Ethoxyethoxy)ethyl acetate	112-15-2	0.32	--	$3.09 \times 10^4$	$5.62 \times 10^{-8}$	$7.22 \times 10^{-10}$	$2.29 \times 10^{-8}$

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2-(Dibutylamino)ethanol	102-81-8	2.01	2.65	3,297	$9.70 \times 10^{-9}$	$1.02 \times 10^{-8}$	--
2-(Hydroxymethylamino)ethanol	34375-28-5	-1.53	--	$1.00 \times 10^6$	$1.62 \times 10^{-12}$	--	--
2-(Thiocyanomethylthio)benzothiazole	21564-17-0	3.12	3.3	41.67	$6.49 \times 10^{-12}$	--	--
2,2'-(Diazene-1,2-diyl)diethane-1,1-diyl)bis-4,5-dihydro-1H-imidazole dihydrochloride	27776-21-2	2.12	--	193.3	$3.11 \times 10^{-14}$	--	--
2,2'-(Octadecylimino)diethanol	10213-78-2	6.85	--	0.08076	$1.06 \times 10^{-8}$	$7.39 \times 10^{-12}$	--
2,2'-[Ethane-1,2-diylbis(oxy)]diethanamine	929-59-9	-2.17	--	$1.00 \times 10^6$	$2.50 \times 10^{-13}$	$8.10 \times 10^{-16}$	--
2,2'-Azobis(2-amidinopropane) dihydrochloride	2997-92-4	-3.28	--	$1.00 \times 10^6$	$1.21 \times 10^{-14}$	--	--
2,2-Dibromo-3-nitrilopropionamide	10222-01-2	1.01	0.82	2,841	$6.16 \times 10^{-14}$	--	$1.91 \times 10^{-8}$
2,2-Dibromopropanediamide	73003-80-2	0.37	--	$1.00 \times 10^4$	$3.58 \times 10^{-14}$	--	--
2,4-Hexadienoic acid, potassium salt, (2E,4E)-	24634-61-5	1.62	1.33	$1.94 \times 10^4$	$5.72 \times 10^{-7}$	$4.99 \times 10^{-8}$	--

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2,6,8-Trimethyl-4-nonanol	123-17-1	4.48	--	24.97	$9.63 \times 10^{-5}$	$4.45 \times 10^{-4}$	--
2-Acrylamido-2-methyl-1-propanesulfonic acid	15214-89-8	-2.19	--	$1.00 \times 10^6$	$5.18 \times 10^{-15}$	--	--
2-Amino-2-methylpropan-1-ol	124-68-5	-0.74	--	$1.00 \times 10^6$	$6.48 \times 10^{-10}$	--	--
2-Aminoethanol hydrochloride	2002-24-6	-1.61	-1.31	$1.00 \times 10^6$	$3.68 \times 10^{-10}$	$9.96 \times 10^{-11}$	--
2-Bromo-3-nitrilopropionamide	1113-55-9	-0.31	--	3,274	$5.35 \times 10^{-13}$	--	--
2-Butanone oxime	96-29-7	1.69	0.63	$3.66 \times 10^4$	$1.04 \times 10^{-5}$	--	--
2-Butoxy-1-propanol	15821-83-7	0.98	--	$4.21 \times 10^4$	$1.30 \times 10^{-7}$	$4.88 \times 10^{-8}$	--
2-Butoxyethanol	111-76-2	0.57	0.83	$6.45 \times 10^4$	$9.79 \times 10^{-8}$	$2.08 \times 10^{-8}$	$1.60 \times 10^{-6}$
2-Dodecylbenzenesulfonic acid- N-(2-aminoethyl)ethane-1,2-diamine(1:1)	40139-72-8	4.78	--	0.7032	$6.27 \times 10^{-8}$	--	--
2-Ethoxyethanol	110-80-5	-0.42	-0.32	$7.55 \times 10^5$	$5.56 \times 10^{-8}$	$1.04 \times 10^{-8}$	$4.70 \times 10^{-7}$
2-Ethoxynaphthalene	93-18-5	3.74	--	38.32	$4.13 \times 10^{-5}$	$4.06 \times 10^{-4}$	--

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2-Ethyl-1-hexanol	104-76-7	2.73	--	1,379	$3.10 \times 10^{-5}$	$4.66 \times 10^{-5}$	$2.65 \times 10^{-5}$
2-Ethyl-2-hexenal	645-62-5	2.62	--	548.6	$2.06 \times 10^{-4}$	$4.88 \times 10^{-4}$	--
2-Ethylhexyl benzoate	5444-75-7	5.19	--	1.061	$2.52 \times 10^{-4}$	$2.34 \times 10^{-4}$	--
2-Hydroxyethyl acrylate	818-61-1	-0.25	-0.21	$5.07 \times 10^5$	$4.49 \times 10^{-9}$	$7.22 \times 10^{-10}$	--
2-Hydroxyethylammonium hydrogen sulphite	13427-63-9	-1.61	-1.31	$1.00 \times 10^6$	$3.68 \times 10^{-10}$	$9.96 \times 10^{-11}$	--
2-Hydroxy-N,N-bis(2-hydroxyethyl)-N-methylethanaminium chloride	7006-59-9	-6.7	--	$1.00 \times 10^6$	$4.78 \times 10^{-19}$	--	--
2-Mercaptoethanol	60-24-2	-0.2	--	$1.94 \times 10^5$	$1.27 \times 10^{-7}$	$3.38 \times 10^{-8}$	$1.80 \times 10^{-7}$
2-Methoxyethanol	109-86-4	-0.91	-0.77	$1.00 \times 10^6$	$4.19 \times 10^{-8}$	$7.73 \times 10^{-9}$	$3.30 \times 10^{-7}$
2-Methyl-1-propanol	78-83-1	0.77	0.76	$9.71 \times 10^4$	$9.99 \times 10^{-6}$	$1.17 \times 10^{-5}$	$9.78 \times 10^{-6}$
2-Methyl-2,4-pentanediol	107-41-5	0.58	--	$3.26 \times 10^4$	$4.06 \times 10^{-7}$	$3.97 \times 10^{-10}$	--
2-Methyl-3(2H)-isothiazolone	2682-20-4	-0.83	--	$5.37 \times 10^5$	$4.96 \times 10^{-8}$	--	--

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2-Methyl-3-butyn-2-ol	115-19-5	0.45	0.28	$2.40 \times 10^5$	$1.04 \times 10^{-6}$	--	$3.91 \times 10^{-6}$
2-Methylbutane	78-78-4	2.72	--	184.6	1.29	1.44	1.40
2-Methylquinoline hydrochloride	62763-89-7	2.69	2.59	498.5	$7.60 \times 10^{-7}$	$2.13 \times 10^{-6}$	--
2-Phosphono-1,2,4-butanetricarboxylic acid	37971-36-1	-1.66	--	$1.00 \times 10^6$	$1.17 \times 10^{-26}$	--	--
2-Phosphonobutane-1,2,4-tricarboxylic acid, potassium salt (1:x)	93858-78-7	-1.66	--	$1.00 \times 10^6$	$1.17 \times 10^{-26}$	--	--
2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester	13533-05-6	-0.52	-0.3	$3.99 \times 10^5$	$6.98 \times 10^{-11}$	$1.54 \times 10^{-12}$	--
3-(Dimethylamino)propylamine	109-55-7	-0.45	--	$1.00 \times 10^6$	$6.62 \times 10^{-9}$	$4.45 \times 10^{-9}$	--
3,4,4-Trimethyloxazolidine	75673-43-7	0.13	--	$8.22 \times 10^5$	$6.63 \times 10^{-6}$	--	--
3,5,7-Triazatricyclo(3.3.1.1 <sup>3,7</sup> )decane, 1-(3-chloro-2-propenyl)-, chloride, (Z)-	51229-78-8	-5.92	--	$1.00 \times 10^6$	$1.76 \times 10^{-8}$	--	--
3,7-Dimethyl-2,6-octadienal	5392-40-5	3.45	--	84.71	$3.76 \times 10^{-4}$	$4.35 \times 10^{-5}$	--

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3-Hydroxybutanal	107-89-1	-0.72	--	$1.00 \times 10^6$	$4.37 \times 10^{-9}$	$2.28 \times 10^{-9}$	--
3-Methoxypropylamine	5332-73-0	-0.42	--	$1.00 \times 10^6$	$1.56 \times 10^{-7}$	$1.94 \times 10^{-8}$	--
3-Phenylprop-2-enal	104-55-2	1.82	1.9	2,150	$1.60 \times 10^{-6}$	$3.38 \times 10^{-7}$	--
4,4-Dimethyloxazolidine	51200-87-4	-0.08	--	$1.00 \times 10^6$	$3.02 \times 10^{-6}$	--	--
4,6-Dimethyl-2-heptanone	19549-80-5	2.56	--	528.8	$2.71 \times 10^{-4}$	$4.55 \times 10^{-4}$	--
4-[Abieta-8,11,13-trien-18-yl(3-oxo-3-phenylpropyl)amino]butan-2-one hydrochloride	143106-84-7	7.72	--	0.002229	$2.49 \times 10^{-12}$	$1.20 \times 10^{-14}$	--
4-Ethyl-1-yn-3-ol	5877-42-9	2.87	--	833.9	$4.27 \times 10^{-6}$	--	--
4-Hydroxy-3-methoxybenzaldehyde	121-33-5	1.05	1.21	6,875	$8.27 \times 10^{-11}$	$2.81 \times 10^{-9}$	$2.15 \times 10^{-9}$
4-Methoxybenzyl formate	122-91-8	1.61	--	2,679	$1.15 \times 10^{-6}$	$2.13 \times 10^{-6}$	--
4-Methoxyphenol	150-76-5	1.59	1.58	$1.65 \times 10^4$	$3.32 \times 10^{-8}$	$5.35 \times 10^{-7}$	--
4-Methyl-2-pentanol	108-11-2	1.68	--	$1.38 \times 10^4$	$1.76 \times 10^{-5}$	$3.88 \times 10^{-5}$	$4.45 \times 10^{-5}$

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4-Methyl-2-pentanone	108-10-1	1.16	1.31	8,888	$1.16 \times 10^{-4}$	$1.34 \times 10^{-4}$	$1.38 \times 10^{-4}$
4-Nonylphenol	104-40-5	5.99	5.76	1.57	$5.97 \times 10^{-6}$	$1.23 \times 10^{-5}$	$3.40 \times 10^{-5}$
5-Chloro-2-methyl-3(2H)-isothiazolone	26172-55-4	-0.34	--	$1.49 \times 10^5$	$3.57 \times 10^{-8}$	--	--
Acetaldehyde	75-07-0	-0.17	-0.34	$2.57 \times 10^5$	$6.78 \times 10^{-5}$	$6.00 \times 10^{-5}$	$6.67 \times 10^{-5}$
Acetic acid	64-19-7	0.09	-0.17	$4.76 \times 10^5$	$5.48 \times 10^{-7}$	$2.94 \times 10^{-7}$	$1.00 \times 10^{-7}$
Acetic acid, C6-8-branched alkyl esters	90438-79-2	3.25	--	117.8	$9.60 \times 10^{-4}$	$1.07 \times 10^{-3}$	--
Acetic acid, hydroxy-, reaction products with triethanolamine	68442-62-6	-2.48	-1	$1.00 \times 10^6$	$4.18 \times 10^{-12}$	$3.38 \times 10^{-19}$	$7.05 \times 10^{-13}$
Acetic acid, mercapto-, monoammonium salt	5421-46-5	0.03	0.09	$2.56 \times 10^5$	$1.94 \times 10^{-8}$	--	--
Acetic anhydride	108-24-7	-0.58	--	$3.59 \times 10^5$	$3.57 \times 10^{-5}$	--	$5.71 \times 10^{-6}$
Acetone	67-64-1	-0.24	-0.24	$2.20 \times 10^5$	$4.96 \times 10^{-5}$	$3.97 \times 10^{-5}$	$3.50 \times 10^{-5}$
Acetonitrile, 2,2',2''-nitrilotris-	7327-60-8	-1.39	--	$1.00 \times 10^6$	$2.61 \times 10^{-15}$	--	--

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Acetophenone	98-86-2	1.67	1.58	4,484	$9.81 \times 10^{-6}$	$1.09 \times 10^{-5}$	$1.04 \times 10^{-5}$
Acetyltriethyl citrate	77-89-4	1.34	--	688.2	$6.91 \times 10^{-11}$	--	--
Acrolein	107-02-8	0.19	-0.01	$1.40 \times 10^5$	$3.58 \times 10^{-5}$	$1.94 \times 10^{-5}$	$1.22 \times 10^{-4}$
Acrylamide	79-06-1	-0.81	-0.67	$5.04 \times 10^5$	$5.90 \times 10^{-9}$	--	$1.70 \times 10^{-9}$
Acrylic acid	79-10-7	0.44	0.35	$1.68 \times 10^5$	$2.89 \times 10^{-7}$	$1.17 \times 10^{-7}$	$3.70 \times 10^{-7}$
Acrylic acid, with sodium-2-acrylamido-2-methyl-1-propanesulfonate and sodium phosphinate	110224-99-2	-2.19	--	$1.00 \times 10^6$	$5.18 \times 10^{-15}$	--	--
Alcohols, C10-12, ethoxylated	67254-71-1	5.47	--	0.9301	$1.95 \times 10^{-2}$	$2.03 \times 10^{-2}$	--
Alcohols, C11-14-iso-, C13-rich	68526-86-3	5.19	--	5.237	$1.28 \times 10^{-4}$	$2.62 \times 10^{-4}$	--
Alcohols, C11-14-iso-, C13-rich, ethoxylated	78330-21-9	4.91	--	5.237	$1.25 \times 10^{-6}$	$7.73 \times 10^{-7}$	--
Alcohols, C12-13, ethoxylated	66455-14-9	5.96	--	0.2995	$2.58 \times 10^{-2}$	$2.87 \times 10^{-2}$	--

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Alcohols, C12-14, ethoxylated propoxylated	68439-51-0	6.67	--	0.02971	$7.08 \times 10^{-4}$	$1.23 \times 10^{-4}$	--
Alcohols, C12-14-secondary	126950-60-5	5.19	--	5.237	$1.28 \times 10^{-4}$	$3.62 \times 10^{-4}$	--
Alcohols, C12-16, ethoxylated	68551-12-2	6.45	--	0.09603	$3.43 \times 10^{-2}$	$4.06 \times 10^{-2}$	--
Alcohols, C14-15, ethoxylated	68951-67-7	7.43	--	0.009765	$6.04 \times 10^{-2}$	$8.10 \times 10^{-2}$	--
Alcohols, C6-12, ethoxylated	68439-45-2	4.49	--	8.832	$1.10 \times 10^{-2}$	$1.02 \times 10^{-2}$	--
Alcohols, C7-9-iso-, C8-rich, ethoxylated	78330-19-5	2.46	--	1,513	$3.04 \times 10^{-7}$	$1.38 \times 10^{-7}$	--
Alcohols, C9-11, ethoxylated	68439-46-3	4.98	--	2.874	$1.47 \times 10^{-2}$	$1.44 \times 10^{-2}$	--
Alcohols, C9-11-iso-, C10-rich, ethoxylated	78330-20-8	4.9	--	3.321	$1.47 \times 10^{-2}$	$2.39 \times 10^{-2}$	--
Alkanes, C12-14-iso-	68551-19-9	6.65	--	0.03173	$1.24 \times 10^1$	$2.28 \times 10^1$	--
Alkanes, C13-16-iso-	68551-20-2	7.63	--	0.003311	$2.19 \times 10^1$	$4.55 \times 10^1$	--
Alkenes, C>10 alpha-	64743-02-8	8.55	--	0.0003941	8.09	$2.39 \times 10^1$	--

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Alkyl* dimethyl ethylbenzyl ammonium chloride *(50%C12, 30%C14, 17%C16, 3%C18)	85409-23-0_1	3.97	--	3.23	$1.11 \times 10^{-11}$	--	--
Alkyl* dimethyl ethylbenzyl ammonium chloride *(60%C14, 30%C16, 5%C12, 5%C18)	68956-79-6	4.95	--	0.3172	$1.96 \times 10^{-11}$	--	--
Alkylbenzenesulfonate, linear	42615-29-2	4.71	--	0.8126	$6.27 \times 10^{-8}$	--	--
alpha-Lactose monohydrate	5989-81-1	-5.12	--	$1.00 \times 10^6$	$4.47 \times 10^{-22}$	$9.81 \times 10^{-45}$	--
alpha-Terpineol	98-55-5	3.33	2.98	371.7	$1.58 \times 10^{-5}$	$3.15 \times 10^{-6}$	$1.22 \times 10^{-5}$
Amaranth	915-67-3	1.63	--	1.789	$1.49 \times 10^{-30}$	--	--
Aminotrimethylene phosphonic acid	6419-19-8	-5.45	-3.53	$1.00 \times 10^6$	$1.65 \times 10^{-34}$	--	--
Ammonium acetate	631-61-8	0.09	-0.17	$4.76 \times 10^5$	$5.48 \times 10^{-7}$	$2.94 \times 10^{-7}$	$1.00 \times 10^{-7}$
Ammonium acrylate	10604-69-0	0.44	0.35	$1.68 \times 10^5$	$2.89 \times 10^{-7}$	$1.17 \times 10^{-7}$	$3.70 \times 10^{-7}$
Ammonium citrate (1:1)	7632-50-0	-1.67	-1.64	$1.00 \times 10^6$	$8.33 \times 10^{-18}$	--	$4.33 \times 10^{-14}$

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Ammonium citrate (2:1)	3012-65-5	-1.67	-1.64	$1.00 \times 10^6$	$8.33 \times 10^{-18}$	--	$4.33 \times 10^{-14}$
Ammonium dodecyl sulfate	2235-54-3	2.42	--	163.7	$1.84 \times 10^{-7}$	--	--
Ammonium hydrogen carbonate	1066-33-7	-0.46	--	$8.42 \times 10^5$	$6.05 \times 10^{-9}$	--	--
Ammonium lactate	515-98-0	-0.65	-0.72	$1.00 \times 10^6$	$1.13 \times 10^{-7}$	--	$8.13 \times 10^{-8}$
Anethole	104-46-1	3.39	--	98.68	$2.56 \times 10^{-4}$	$2.23 \times 10^{-3}$	--
Aniline	62-53-3	1.08	0.9	$2.08 \times 10^4$	$1.90 \times 10^{-6}$	$2.18 \times 10^{-6}$	$2.02 \times 10^{-6}$
Benactyzine hydrochloride	57-37-4	2.89	--	292.1	$2.07 \times 10^{-10}$	--	--
Benzamorf	12068-08-5	4.71	--	0.8126	$6.27 \times 10^{-8}$	--	--
Benzene	71-43-2	1.99	2.13	2,000	$5.39 \times 10^{-3}$	$5.35 \times 10^{-3}$	$5.55 \times 10^{-3}$
Benzene, C10-16-alkyl derivatives	68648-87-3	8.43	9.36	0.0002099	$1.78 \times 10^{-1}$	$3.97 \times 10^{-1}$	--
Benzenesulfonic acid	98-11-3	-1.17	--	$6.90 \times 10^5$	$2.52 \times 10^{-9}$	--	--
Benzenesulfonic acid, (1-methylethyl)-,	37953-05-2	0.29	--	$2.46 \times 10^4$	$4.89 \times 10^{-9}$	--	--

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Benzenesulfonic acid, (1-methylethyl)-, ammonium salt	37475-88-0	0.29	--	$2.46 \times 10^4$	$4.89 \times 10^{-9}$	--	--
Benzenesulfonic acid, (1-methylethyl)-, sodium salt	28348-53-0	0.29	--	$2.46 \times 10^4$	$4.89 \times 10^{-9}$	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, compounds with cyclohexylamine	255043-08-4	4.71	--	0.8126	$6.27 \times 10^{-8}$	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, compounds with triethanolamine	68584-25-8	5.2	--	0.255	$8.32 \times 10^{-8}$	--	--
Benzenesulfonic acid, C10-16-alkyl derivatives, potassium salts	68584-27-0	5.2	--	0.255	$8.32 \times 10^{-8}$	--	--
Benzenesulfonic acid, dodecyl-, branched, compounds with 2-propanamine	90218-35-2	4.49	--	1.254	$6.27 \times 10^{-8}$	--	--
Benzenesulfonic acid, mono-C10-16-alkyl derivatives, sodium salts	68081-81-2	4.22	--	2.584	$4.72 \times 10^{-8}$	--	--
Benzoic acid	65-85-0	1.87	1.87	2,493	$1.08 \times 10^{-7}$	$4.55 \times 10^{-8}$	$3.81 \times 10^{-8}$

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm-m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Benzyl chloride	100-44-7	2.79	2.3	1,030	$2.09 \times 10^{-3}$	$3.97 \times 10^{-4}$	$4.12 \times 10^{-4}$
Benzyltrimethylammonium chloride	139-07-1	2.93	--	36.47	$7.61 \times 10^{-12}$	--	--
Benzylhexadecyldimethylammonium chloride	122-18-9	4.89	--	0.3543	$2.36 \times 10^{-11}$	--	--
Benzyltrimethylammonium chloride	56-93-9	-2.47	--	$1.00 \times 10^6$	$3.37 \times 10^{-13}$	--	--
Bicine	150-25-4	-3.27	--	$3.52 \times 10^5$	$1.28 \times 10^{-14}$	--	--
Bis(1-methylethyl)naphthalenesulfonic acid, cyclohexylamine salt	68425-61-6	2.92	--	43.36	$9.29 \times 10^{-10}$	--	--
Bis(2-chloroethyl) ether	111-44-4	1.56	1.29	6,435	$1.89 \times 10^{-4}$	$4.15 \times 10^{-7}$	$1.70 \times 10^{-5}$
Bisphenol A	80-05-7	3.64	3.32	172.7	$9.16 \times 10^{-12}$	--	--
Bronopol	52-51-7	-1.51	--	$8.37 \times 10^5$	$6.35 \times 10^{-21}$	--	--
Butane	106-97-8	2.31	2.89	135.6	$9.69 \times 10^{-1}$	$8.48 \times 10^{-1}$	$9.50 \times 10^{-1}$

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Butanedioic acid, sulfo-, 1,4-bis(1,3-dimethylbutyl) ester, sodium salt	2373-38-8	3.98	--	0.1733	$1.61 \times 10^{-12}$	--	--
Butene	25167-67-3	2.17	2.4	354.8	$2.03 \times 10^{-1}$	$2.68 \times 10^{-1}$	$2.33 \times 10^{-1}$
Butyl glycidyl ether	2426-08-6	1.08	0.63	$2.66 \times 10^4$	$4.37 \times 10^{-6}$	$5.23 \times 10^{-7}$	$2.47 \times 10^{-5}$
Butyl lactate	138-22-7	0.8	--	$5.30 \times 10^4$	$8.49 \times 10^{-5}$	--	$1.92 \times 10^{-6}$
Butyryl trihexyl citrate	82469-79-2	8.21	--	$5.56 \times 10^{-5}$	$3.65 \times 10^{-9}$	--	--
C.I. Acid Red 1	3734-67-6	0.51	--	6.157	$3.73 \times 10^{-29}$	--	--
C.I. Acid Violet 12, disodium salt	6625-46-3	0.59	--	3.379	$2.21 \times 10^{-30}$	--	--
C.I. Pigment Red 5	6410-41-9	7.65	--	$4.38 \times 10^{-5}$	$4.36 \times 10^{-21}$	--	--
C.I. Solvent Red 26	4477-79-6	9.27	--	$5.68 \times 10^{-5}$	$5.48 \times 10^{-13}$	$4.66 \times 10^{-13}$	--
C10-16-Alkyldimethylamines oxides	70592-80-2	2.87	--	89.63	$1.14 \times 10^{-13}$	--	--
C10-C16 Ethoxylated alcohol	68002-97-1	4.99	--	4.532	$1.25 \times 10^{-6}$	$4.66 \times 10^{-7}$	--

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
C12-14 tert-Alkyl ethoxylated amines	73138-27-9	3.4	--	264.2	$1.29 \times 10^{-10}$	--	--
Calcium dodecylbenzene sulfonate	26264-06-2	4.71	--	0.8126	$6.27 \times 10^{-8}$	--	--
Camphor	76-22-2	3.04	2.38	339.1	$7.00 \times 10^{-5}$	--	$8.10 \times 10^{-5}$
Carbon dioxide	124-38-9	0.83	0.83	$2.57 \times 10^4$	$1.52 \times 10^{-2}$	--	$1.52 \times 10^{-2}$
Carbonic acid, dipotassium salt	584-08-7	-0.46	--	$8.42 \times 10^5$	$6.05 \times 10^{-9}$	--	--
Choline bicarbonate	78-73-9	-5.16	--	$1.00 \times 10^6$	$2.03 \times 10^{-16}$	--	--
Choline chloride	67-48-1	-5.16	--	$1.00 \times 10^6$	$2.03 \times 10^{-16}$	--	--
Citric acid	77-92-9	-1.67	-1.64	$1.00 \times 10^6$	$8.33 \times 10^{-18}$	--	$4.33 \times 10^{-14}$
Citronellol	106-22-9	3.56	3.91	105.5	$5.68 \times 10^{-5}$	$2.13 \times 10^{-5}$	--
Coconut trimethylammonium chloride	61789-18-2	1.22	--	2,816	$9.42 \times 10^{-11}$	--	--
Coumarin	91-64-5	1.51	1.39	5,126	$6.95 \times 10^{-6}$	--	$9.92 \times 10^{-8}$
Cumene	98-82-8	3.45	3.66	75.03	$1.05 \times 10^{-2}$	$1.23 \times 10^{-2}$	$1.15 \times 10^{-2}$

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Cyclohexane	110-82-7	3.18	3.44	43.02	$2.55 \times 10^{-1}$	$1.94 \times 10^{-1}$	$1.50 \times 10^{-1}$
Cyclohexanol	108-93-0	1.64	1.23	$3.37 \times 10^4$	$4.90 \times 10^{-6}$	$3.70 \times 10^{-6}$	$4.40 \times 10^{-6}$
Cyclohexanone	108-94-1	1.13	0.81	$2.41 \times 10^4$	$5.11 \times 10^{-5}$	$1.28 \times 10^{-5}$	$9.00 \times 10^{-6}$
Cyclohexylamine sulfate	19834-02-7	1.63	1.49	$6.40 \times 10^4$	$1.38 \times 10^{-5}$	--	$4.16 \times 10^{-6}$
D&C Red no. 28	18472-87-2	9.62	--	$1.64 \times 10^{-8}$	$6.37 \times 10^{-21}$	--	--
D&C Red no. 33	3567-66-6	0.48	--	11.87	$1.15 \times 10^{-26}$	--	--
Daidzein	486-66-8	2.55	--	568.4	$3.91 \times 10^{-16}$	--	--
Dapsone	80-08-0	0.77	0.97	3,589	$3.11 \times 10^{-14}$	--	--
Dazomet	533-74-4	0.94	0.63	$1.94 \times 10^4$	$2.84 \times 10^{-3}$	--	$4.98 \times 10^{-10}$
Decyldimethylamine	1120-24-7	4.46	--	82.23	$4.68 \times 10^{-4}$	$2.45 \times 10^{-3}$	--
D-Glucitol	50-70-4	-3.01	-2.2	$1.00 \times 10^6$	$7.26 \times 10^{-13}$	$2.94 \times 10^{-29}$	--
D-Gluconic acid	526-95-4	-1.87	--	$1.00 \times 10^6$	$4.74 \times 10^{-13}$	--	--

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D-Glucopyranoside, methyl	3149-68-6	-2.5	--	$1.00 \times 10^6$	$1.56 \times 10^{-14}$	$2.23 \times 10^{-24}$	--
D-Glucose	50-99-7	-2.89	-3.24	$1.00 \times 10^6$	$9.72 \times 10^{-15}$	$1.62 \times 10^{-26}$	--
Di(2-ethylhexyl) phthalate	117-81-7	8.39	7.6	0.001132	$1.18 \times 10^{-5}$	$1.02 \times 10^{-5}$	$2.70 \times 10^{-7}$
Dibromoacetonitrile	3252-43-5	0.47	--	9,600	$4.06 \times 10^{-7}$	--	--
Dichloromethane	75-09-2	1.34	1.25	$1.10 \times 10^4$	$9.14 \times 10^{-3}$	$3.01 \times 10^{-3}$	$3.25 \times 10^{-3}$
Didecyldimethylammonium chloride	7173-51-5	4.66	--	0.9	$6.85 \times 10^{-10}$	--	--
Diethanolamine	111-42-2	-1.71	-1.43	$1.00 \times 10^6$	$3.92 \times 10^{-11}$	$3.46 \times 10^{-15}$	$3.87 \times 10^{-11}$
Diethylbenzene	25340-17-4	4.07	3.72	58.86	$1.16 \times 10^{-2}$	$1.47 \times 10^{-2}$	$2.61 \times 10^{-3}$
Diethylene glycol	111-46-6	-1.47	--	$1.00 \times 10^6$	$2.03 \times 10^{-9}$	$1.20 \times 10^{-13}$	--
Diethylene glycol monomethyl ether	111-77-3	-1.18	--	$1.00 \times 10^6$	$6.50 \times 10^{-10}$	$1.65 \times 10^{-11}$	--
Diethylenetriamine	111-40-0	-2.13	--	$1.00 \times 10^6$	$3.10 \times 10^{-13}$	$1.09 \times 10^{-14}$	--
Diisobutyl ketone	108-83-8	2.56	--	528.8	$2.71 \times 10^{-4}$	$4.55 \times 10^{-4}$	$1.17 \times 10^{-4}$

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Diisopropanolamine	110-97-4	-0.88	-0.82	$1.00 \times 10^6$	$6.91 \times 10^{-11}$	$1.90 \times 10^{-14}$	--
Diisopropylnaphthalene	38640-62-9	6.08	--	0.2421	$1.99 \times 10^{-3}$	$1.94 \times 10^{-3}$	--
Dimethyl adipate	627-93-0	1.39	1.03	7,749	$9.77 \times 10^{-7}$	$1.28 \times 10^{-7}$	$2.31 \times 10^{-6}$
Dimethyl glutarate	1119-40-0	0.9	0.62	$2.02 \times 10^4$	$7.36 \times 10^{-7}$	$9.09 \times 10^{-8}$	$6.43 \times 10^{-7}$
Dimethyl succinate	106-65-0	0.4	0.35	$3.96 \times 10^4$	$5.54 \times 10^{-7}$	$6.43 \times 10^{-8}$	--
Dimethylaminoethanol	108-01-0	-0.94	--	$1.00 \times 10^6$	$1.77 \times 10^{-9}$	$1.77 \times 10^{-9}$	$3.73 \times 10^{-7}$
Dimethyldiallylammonium chloride	7398-69-8	-2.49	--	$1.00 \times 10^6$	$7.20 \times 10^{-12}$	--	--
Diphenyl oxide	101-84-8	4.05	4.21	15.58	$1.18 \times 10^{-4}$	$2.81 \times 10^{-4}$	$2.79 \times 10^{-4}$
Dipropylene glycol	25265-71-8	-0.64	--	$3.11 \times 10^5$	$3.58 \times 10^{-9}$	$6.29 \times 10^{-10}$	--
Di-sec-butylphenol	31291-60-8	5.41	--	3.723	$3.74 \times 10^{-6}$	$6.89 \times 10^{-6}$	--
Disodium dodecyl(sulphonatophenoxy)benzenesulp honate	28519-02-0	5.05	--	0.0353	$6.40 \times 10^{-16}$	--	--

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Disodium ethylenediaminediacetate	38011-25-5	-4.79	--	$1.00 \times 10^6$	$1.10 \times 10^{-16}$	--	--
Disodium ethylenediaminetetraacetate dihydrate	6381-92-6	-3.86	--	$2.28 \times 10^5$	$1.17 \times 10^{-23}$	--	$5.77 \times 10^{-16}$
D-Lactic acid	10326-41-7	-0.65	-0.72	$1.00 \times 10^6$	$1.13 \times 10^{-7}$	--	$8.13 \times 10^{-8}$
D-Limonene	5989-27-5	4.83	4.57	4.581	$3.80 \times 10^{-1}$	--	$3.19 \times 10^{-2}$
Docusate sodium	577-11-7	6.1	--	0.001227	$5.00 \times 10^{-12}$	--	--
Dodecane	112-40-3	6.23	6.1	0.1099	9.35	$1.34 \times 10^1$	8.18
Dodecylbenzene	123-01-3	7.94	8.65	0.001015	$1.34 \times 10^{-1}$	$2.81 \times 10^{-1}$	--
Dodecylbenzenesulfonic acid	27176-87-0	4.71	--	0.8126	$6.27 \times 10^{-8}$	--	--
Dodecylbenzenesulfonic acid, monoethanolamine salt	26836-07-7	4.71	--	0.8126	$6.27 \times 10^{-8}$	--	--
Epichlorohydrin	106-89-8	0.63	0.45	$5.06 \times 10^4$	$5.62 \times 10^{-5}$	$2.62 \times 10^{-6}$	$3.04 \times 10^{-5}$

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Ethanaminium, N,N,N-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride	44992-01-0	-3.1	--	$1.00 \times 10^6$	$6.96 \times 10^{-15}$	--	--
Ethane	74-84-0	1.32	1.81	938.6	$5.50 \times 10^{-1}$	$4.25 \times 10^{-1}$	$5.00 \times 10^{-1}$
Ethanol	64-17-5	-0.14	-0.31	$7.92 \times 10^5$	$5.67 \times 10^{-6}$	$4.88 \times 10^{-6}$	$5.00 \times 10^{-6}$
Ethanol, 2,2',2''-nitritotris-, tris(dihydrogen phosphate) (ester), sodium salt	68171-29-9	-3.13	--	$1.00 \times 10^6$	$3.08 \times 10^{-36}$	--	--
Ethanol, 2-[2-[2-(tridecyloxy)ethoxy]ethoxy]-, hydrogen sulfate, sodium salt	25446-78-0	2.09	--	42	$9.15 \times 10^{-13}$	--	--
Ethanolamine	141-43-5	-1.61	-1.31	$1.00 \times 10^6$	$3.68 \times 10^{-10}$	$9.96 \times 10^{-11}$	--
Ethoxylated dodecyl alcohol	9002-92-0	4.5	--	14.19	$9.45 \times 10^{-7}$	$3.30 \times 10^{-7}$	--
Ethyl acetate	141-78-6	0.86	0.73	$2.99 \times 10^4$	$2.33 \times 10^{-4}$	$1.58 \times 10^{-4}$	$1.34 \times 10^{-4}$
Ethyl acetoacetate	141-97-9	-0.2	0.25	$5.62 \times 10^4$	$1.57 \times 10^{-7}$	--	$1.20 \times 10^{-6}$
Ethyl benzoate	93-89-0	2.32	2.64	421.5	$4.61 \times 10^{-5}$	$2.45 \times 10^{-5}$	$7.33 \times 10^{-5}$

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		Estimated	Measured		Bond method	Group method 25	Measured
Ethyl lactate	97-64-3	-0.18	--	$4.73 \times 10^5$	$4.82 \times 10^{-5}$	--	$5.83 \times 10^{-7}$
Ethyl salicylate	118-61-6	3.09	2.95	737.1	$6.04 \times 10^{-6}$	$3.01 \times 10^{-9}$	--
Ethylbenzene	100-41-4	3.03	3.15	228.6	$7.89 \times 10^{-3}$	$8.88 \times 10^{-3}$	$7.88 \times 10^{-3}$
Ethylene	74-85-1	1.27	1.13	3,449	$9.78 \times 10^{-2}$	$1.62 \times 10^{-1}$	$2.28 \times 10^{-1}$
Ethylene glycol	107-21-1	-1.2	-1.36	$1.00 \times 10^6$	$1.31 \times 10^{-7}$	$5.60 \times 10^{-11}$	$6.00 \times 10^{-8}$
Ethylene oxide	75-21-8	-0.05	-0.3	$2.37 \times 10^5$	$1.20 \times 10^{-4}$	$5.23 \times 10^{-5}$	$1.48 \times 10^{-4}$
Ethylenediamine	107-15-3	-1.62	-2.04	$1.00 \times 10^6$	$1.03 \times 10^{-9}$	$1.77 \times 10^{-10}$	$1.73 \times 10^{-9}$
Ethylenediaminetetraacetic acid	60-00-4	-3.86	--	$2.28 \times 10^5$	$1.17 \times 10^{-23}$	--	$5.77 \times 10^{-16}$
Ethylenediaminetetraacetic acid tetrasodium salt	64-02-8	-3.86	--	$2.28 \times 10^5$	$1.17 \times 10^{-23}$	--	$5.77 \times 10^{-16}$
Ethylenediaminetetraacetic acid, disodium salt	139-33-3	-3.86	--	$2.28 \times 10^5$	$1.17 \times 10^{-23}$	--	$5.77 \times 10^{-16}$
Ethyne	74-86-2	0.5	0.37	$1.48 \times 10^4$	$2.40 \times 10^{-2}$	$2.45 \times 10^{-2}$	$2.17 \times 10^{-2}$

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Fatty acids, C18-unsaturated, dimers	61788-89-4	14.6	--	$2.31 \times 10^{-10}$	$4.12 \times 10^{-8}$	$9.74 \times 10^{-9}$	--
FD&C Blue no. 1	3844-45-9	-0.15	--	0.2205	$2.25 \times 10^{-35}$	--	--
FD&C Yellow no. 5	1934-21-0	-1.82	--	7.388	$1.31 \times 10^{-28}$	--	--
FD&C Yellow no. 6	2783-94-0	1.4	--	242.7	$3.26 \times 10^{-23}$	--	--
Formaldehyde	50-00-0	0.35	0.35	$5.70 \times 10^4$	$9.29 \times 10^{-5}$	$6.14 \times 10^{-5}$	$3.37 \times 10^{-7}$
Formamide	75-12-7	-1.61	-1.51	$1.00 \times 10^6$	$1.53 \times 10^{-8}$	--	$1.39 \times 10^{-9}$
Formic acid	64-18-6	-0.46	-0.54	$9.55 \times 10^5$	$7.50 \times 10^{-7}$	$5.11 \times 10^{-7}$	$1.67 \times 10^{-7}$
Formic acid, potassium salt	590-29-4	-0.46	-0.54	$9.55 \times 10^5$	$7.50 \times 10^{-7}$	$5.11 \times 10^{-7}$	$1.67 \times 10^{-7}$
Fumaric acid	110-17-8	0.05	-0.48	$1.04 \times 10^5$	$1.35 \times 10^{-12}$	$8.48 \times 10^{-14}$	--
Furfural	98-01-1	0.83	0.41	$5.36 \times 10^4$	$1.34 \times 10^{-5}$	--	$3.77 \times 10^{-6}$
Furfuryl alcohol	98-00-0	0.45	0.28	$2.21 \times 10^5$	$2.17 \times 10^{-7}$	--	$7.86 \times 10^{-8}$
Galantamine hydrobromide	69353-21-5	2.29	--	1,606	$1.70 \times 10^{-13}$	--	--

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Gluconic acid	133-42-6	-1.87	--	$1.00 \times 10^6$	$4.74 \times 10^{-13}$	--	--
Glutaraldehyde	111-30-8	-0.18	--	$1.67 \times 10^5$	$1.10 \times 10^{-7}$	$2.39 \times 10^{-8}$	--
Glycerol	56-81-5	-1.65	-1.76	$1.00 \times 10^6$	$6.35 \times 10^{-9}$	$1.51 \times 10^{-15}$	$1.73 \times 10^{-8}$
Glycine, N-(carboxymethyl)-N-(2-hydroxyethyl)-, disodium salt	135-37-5	-3.04	--	$1.90 \times 10^5$	$3.90 \times 10^{-17}$	--	--
Glycine, N-(hydroxymethyl)-, monosodium salt	70161-44-3	-3.41	--	$7.82 \times 10^5$	$1.80 \times 10^{-12}$	--	--
Glycine, N,N-bis(carboxymethyl)-, trisodium salt	5064-31-3	-3.81	--	$7.39 \times 10^5$	$1.19 \times 10^{-16}$	--	--
Glycine, N-[2-bis(carboxymethyl)amino]ethyl]-N-(2-hydroxyethyl)-, trisodium salt	139-89-9	-4.09	--	$4.31 \times 10^5$	$3.81 \times 10^{-24}$	--	--
Glycolic acid	79-14-1	-1.07	-1.11	$1.00 \times 10^6$	$8.54 \times 10^{-8}$	$6.29 \times 10^{-11}$	--
Glycolic acid sodium salt	2836-32-0	-1.07	-1.11	$1.00 \times 10^6$	$8.54 \times 10^{-8}$	$6.29 \times 10^{-11}$	--
Glyoxal	107-22-2	-1.66	--	$1.00 \times 10^6$	$3.70 \times 10^{-7}$	--	$3.33 \times 10^{-9}$

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm·m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Glyoxylic acid	298-12-4	-1.4	--	$1.00 \times 10^6$	$2.98 \times 10^{-9}$	--	--
Heptane	142-82-5	3.78	4.66	3.554	2.27	2.39	2.00
Hexadecyltrimethylammonium bromide	57-09-0	3.18	--	28.77	$2.93 \times 10^{-10}$	--	--
Hexane	110-54-3	3.29	3.9	17.24	1.71	1.69	1.80
Hexanedioic acid	124-04-9	0.23	0.08	$1.67 \times 10^5$	$9.53 \times 10^{-12}$	$8.10 \times 10^{-13}$	$4.71 \times 10^{-12}$
Hydroxyvaleric acid	1619-16-5	3.31	--	282.1	--	--	--
Indole	120-72-9	2.05	2.14	1,529	$8.86 \times 10^{-7}$	$1.99 \times 10^{-6}$	$5.28 \times 10^{-7}$
Isoascorbic acid	89-65-6	-1.88	-1.85	$1.00 \times 10^6$	$4.07 \times 10^{-8}$	--	--
Isobutane	75-28-5	2.23	2.76	175.1	$9.69 \times 10^{-1}$	1.02	1.19
Isobutene	115-11-7	2.23	2.34	399.2	$2.40 \times 10^{-1}$	$2.34 \times 10^{-1}$	$2.18 \times 10^{-1}$
Isooctanol	26952-21-6	2.73	--	1,379	$3.10 \times 10^{-5}$	$4.66 \times 10^{-5}$	$9.21 \times 10^{-5}$
Isopentyl alcohol	123-51-3	1.26	1.16	$4.16 \times 10^4$	$1.33 \times 10^{-5}$	$1.65 \times 10^{-5}$	$1.41 \times 10^{-5}$

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Isopropanol	67-63-0	0.28	0.05	$4.02 \times 10^5$	$7.52 \times 10^{-6}$	$1.14 \times 10^{-5}$	$8.10 \times 10^{-6}$
Isopropanolamine dodecylbenzene	42504-46-1	7.94	8.65	0.001015	$1.34 \times 10^{-1}$	$2.81 \times 10^{-1}$	--
Isopropylamine	75-31-0	0.27	0.26	$8.38 \times 10^5$	$1.34 \times 10^{-5}$	--	$4.51 \times 10^{-5}$
Isoquinoline	119-65-3	2.14	2.08	1,551	$6.88 \times 10^{-7}$	$4.15 \times 10^{-7}$	--
Isoquinoline, reaction products with benzyl chloride and quinoline	68909-80-8	2.14	2.08	1,551	$6.88 \times 10^{-7}$	$4.15 \times 10^{-7}$	--
Isoquinolinium, 2-(phenylmethyl)-, chloride	35674-56-7	4.4	--	6.02	$1.19 \times 10^{-6}$	--	--
Lactic acid	50-21-5	-0.65	-0.72	$1.00 \times 10^6$	$1.13 \times 10^{-7}$	--	$8.13 \times 10^{-8}$
Lactose	63-42-3	-5.12	--	$1.00 \times 10^6$	$4.47 \times 10^{-22}$	$9.81 \times 10^{-45}$	--
Lauryl hydroxysultaine	13197-76-7	-1.3	--	$7.71 \times 10^4$	$1.04 \times 10^{-21}$	--	--
L-Dilactide	4511-42-6	1.65	--	3,165	$1.22 \times 10^{-5}$	--	--
L-Glutamic acid	56-86-0	-3.83	-3.69	$9.42 \times 10^5$	$1.47 \times 10^{-14}$	--	--

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
L-Lactic acid	79-33-4	-0.65	-0.72	$1.00 \times 10^6$	$1.13 \times 10^{-7}$	--	$8.13 \times 10^{-8}$
Methane	74-82-8	0.78	1.09	2,610	$4.14 \times 10^{-1}$	$6.58 \times 10^{-1}$	$6.58 \times 10^{-1}$
Methanol	67-56-1	-0.63	-0.77	$1.00 \times 10^6$	$4.27 \times 10^{-6}$	$3.62 \times 10^{-6}$	$4.55 \times 10^{-6}$
Methenamine	100-97-0	-4.15	--	$1.00 \times 10^6$	$1.63 \times 10^{-1}$	--	$1.64 \times 10^{-9}$
Methoxyacetic acid	625-45-6	-0.68	--	$1.00 \times 10^6$	$4.54 \times 10^{-8}$	$8.68 \times 10^{-9}$	$6.42 \times 10^{-9}$
Methyl salicylate	119-36-8	2.6	2.55	1,875	$4.55 \times 10^{-6}$	$2.23 \times 10^{-9}$	$9.81 \times 10^{-5}$
Methyl vinyl ketone	78-94-4	0.41	--	$6.06 \times 10^4$	$2.61 \times 10^{-5}$	$1.38 \times 10^{-5}$	$4.65 \times 10^{-5}$
Methylcyclohexane	108-87-2	3.59	3.61	28.4	$3.39 \times 10^{-1}$	$3.30 \times 10^{-1}$	$4.30 \times 10^{-1}$
Methylene bis(thiocyanate)	6317-18-6	0.62	--	$2.72 \times 10^4$	$2.61 \times 10^{-8}$	--	--
Methylenebis(5-methyloxazolidine)	66204-44-2	-0.58	--	$1.00 \times 10^6$	$1.07 \times 10^{-7}$	--	--
Morpholine	110-91-8	-0.56	-0.86	$1.00 \times 10^6$	$1.14 \times 10^{-7}$	$3.22 \times 10^{-9}$	$1.16 \times 10^{-6}$

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Morpholinium, 4-ethyl-4-hexadecyl-, ethyl sulfate	78-21-7	4.54	--	0.9381	$2.66 \times 10^{-12}$	--	--
N-(2-Acryloyloxyethyl)-N-benzyl-N,N-dimethylammonium chloride	46830-22-2	-1.39	--	$4.42 \times 10^5$	$5.62 \times 10^{-16}$	--	--
N-(3-Chloroallyl)hexaminium chloride	4080-31-3	-5.92	--	$1.00 \times 10^6$	$1.76 \times 10^{-8}$	--	--
N,N,N-Trimethyl-3-((1-oxooctadecyl)amino)-1-propanaminium methyl sulfate	19277-88-4	4.38	--	0.7028	$2.28 \times 10^{-16}$	--	--
N,N,N-Trimethyloctadecan-1-aminium chloride	112-03-8	4.17	--	2.862	$5.16 \times 10^{-10}$	--	--
N,N'-Dibutylthiourea	109-46-6	2.57	2.75	2,287	$4.17 \times 10^{-6}$	--	--
N,N-Dimethyldecylamine oxide	2605-79-0	1.4	--	2,722	$4.88 \times 10^{-14}$	--	--
N,N-Dimethylformamide	68-12-2	-0.93	-1.01	$9.78 \times 10^5$	$7.38 \times 10^{-8}$	--	$7.39 \times 10^{-8}$
N,N-Dimethylmethanamine hydrochloride	593-81-7	0.04	0.16	$1.00 \times 10^6$	$3.65 \times 10^{-5}$	$1.28 \times 10^{-4}$	$1.04 \times 10^{-4}$

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
N,N-Dimethyl-methanamine-N-oxide	1184-78-7	-3.02	--	$1.00 \times 10^6$	$3.81 \times 10^{-15}$	--	--
N,N-dimethyloctadecylamine hydrochloride	1613-17-8	8.39	--	0.008882	$4.51 \times 10^{-3}$	$3.88 \times 10^{-2}$	--
N,N'-Methylenebisacrylamide	110-26-9	-1.52	--	$7.01 \times 10^4$	$1.14 \times 10^{-9}$	--	--
Naphthalene	91-20-3	3.17	3.3	142.1	$5.26 \times 10^{-4}$	$3.70 \times 10^{-4}$	$4.40 \times 10^{-4}$
Naphthalenesulfonic acid, bis(1- methylethyl)-	28757-00-8	2.92	--	43.36	$9.29 \times 10^{-10}$	--	--
Naphthalenesulphonic acid, bis (1- methylethyl)-methyl derivatives	99811-86-6	4.02	--	3.45	$1.13 \times 10^{-9}$	--	--
Naphthenic acid ethoxylate	68410-62-8	3.41	--	112.5	$3.62 \times 10^{-8}$	$2.74 \times 10^{-9}$	--
Nitrilotriacetamide	4862-18-4	-4.75	--	$1.00 \times 10^6$	$1.61 \times 10^{-18}$	--	--
Nitrilotriacetic acid	139-13-9	-3.81	--	$7.39 \times 10^5$	$1.19 \times 10^{-16}$	--	--
Nitrilotriacetic acid trisodium monohydrate	18662-53-8	-3.81	--	$7.39 \times 10^5$	$1.19 \times 10^{-16}$	--	--

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		Estimated	Measured		Bond method	Group method 25	Measured
N-Methyl-2-pyrrolidone	872-50-4	-0.11	-0.38	$2.48 \times 10^5$	$3.16 \times 10^{-8}$	--	$3.20 \times 10^{-9}$
N-Methyldiethanolamine	105-59-9	-1.5	--	$1.00 \times 10^6$	$8.61 \times 10^{-11}$	$2.45 \times 10^{-14}$	$3.14 \times 10^{-11}$
N-Methylethanolamine	109-83-1	-1.15	-0.94	$1.00 \times 10^6$	$8.07 \times 10^{-10}$	$2.50 \times 10^{-10}$	--
N-Methyl-N-hydroxyethyl-N-hydroxyethoxyethylamine	68213-98-9	-1.78	--	$1.00 \times 10^6$	$1.34 \times 10^{-12}$	$5.23 \times 10^{-17}$	--
N-Oleyl diethanolamide	13127-82-7	6.63	--	0.1268	$9.35 \times 10^{-9}$	$1.94 \times 10^{-12}$	--
Oleic acid	112-80-1	7.73	7.64	0.01151	$4.48 \times 10^{-5}$	$1.94 \times 10^{-5}$	--
Pentaethylenehexamine	4067-16-7	-3.67	--	$1.00 \times 10^6$	$8.36 \times 10^{-24}$	$2.56 \times 10^{-27}$	--
Pentane	109-66-0	2.8	3.39	49.76	1.29	1.20	1.25
Pentyl acetate	628-63-7	2.34	2.3	996.8	$5.45 \times 10^{-4}$	$4.45 \times 10^{-4}$	$3.88 \times 10^{-4}$
Pentyl butyrate	540-18-1	3.32	--	101.9	$9.60 \times 10^{-4}$	$8.88 \times 10^{-4}$	--
Peracetic acid	79-21-0	-1.07	--	$1.00 \times 10^6$	$1.39 \times 10^{-6}$	--	$2.14 \times 10^{-6}$

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Phenanthrene	85-01-8	4.35	4.46	0.677	$5.13 \times 10^{-5}$	$2.56 \times 10^{-5}$	$4.23 \times 10^{-5}$
Phenol	108-95-2	1.51	1.46	$2.62 \times 10^4$	$5.61 \times 10^{-7}$	$6.58 \times 10^{-7}$	$3.33 \times 10^{-7}$
Phosphonic acid (dimethylamino(methylene))	29712-30-9	-1.9	--	$1.00 \times 10^6$	$1.00 \times 10^{-24}$	--	--
Phosphonic acid, (((2-[(2-hydroxyethyl) (phosphonomethyl)amino)ethyl)imino]bis (methylene))bis-, compd. with 2- aminoethanol	129828-36-0	-6.73	--	$1.00 \times 10^6$	$5.29 \times 10^{-42}$	--	--
Phosphonic acid, (1-hydroxyethylidene) bis-, potassium salt	67953-76-8	-0.01	--	$1.34 \times 10^5$	$9.79 \times 10^{-26}$	--	--
Phosphonic acid, (1-hydroxyethylidene) bis-, tetrasodium salt	3794-83-0	-0.01	--	$1.34 \times 10^5$	$9.79 \times 10^{-26}$	--	--
Phosphonic acid, [[[phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]]tetrakis-	15827-60-8	-9.72	--	$1.00 \times 10^6$	--	--	--

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		Estimated	Measured		Bond method	Group method 25	Measured
Phosphonic acid, [[[phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]]tetrakis-, ammonium salt (1:x)	70714-66-8	-9.72	--	$1.00 \times 10^6$	--	--	--
Phosphonic acid, [[[phosphonomethyl) imino]bis[2,1-ethanediylnitrilobis (methylene)]]]tetrakis-, sodium salt	22042-96-2	-9.72	--	$1.00 \times 10^6$	--	--	--
Phosphonic acid, [[[phosphonomethyl) imino]bis[6,1-hexanediylnitrilobis (methylene)]]]tetrakis-	34690-00-1	-5.79	--	$1.00 \times 10^6$	--	--	--
Phthalic anhydride	85-44-9	2.07	1.6	3,326	$6.35 \times 10^{-6}$	--	$1.63 \times 10^{-8}$
Poly(oxy-1,2-ethanediyl), .alpha.-(octylphenyl)-.omega.-hydroxy-, branched	68987-90-6	5.01	--	3.998	$1.24 \times 10^{-7}$	$1.07 \times 10^{-6}$	--
Potassium acetate	127-08-2	0.09	-0.17	$4.76 \times 10^5$	$5.48 \times 10^{-7}$	$2.94 \times 10^{-7}$	$1.00 \times 10^{-7}$
Potassium oleate	143-18-0	7.73	7.64	0.01151	$4.48 \times 10^{-5}$	$1.94 \times 10^{-5}$	--
Propane	74-98-6	1.81	2.36	368.9	$7.30 \times 10^{-1}$	$6.00 \times 10^{-1}$	$7.07 \times 10^{-1}$

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Propanol, 1(or 2)-(2-methoxymethylethoxy)-	34590-94-8	-0.27	--	$4.27 \times 10^5$	$1.15 \times 10^{-9}$	$1.69 \times 10^{-9}$	--
Propargyl alcohol	107-19-7	-0.42	-0.38	$9.36 \times 10^5$	$5.88 \times 10^{-7}$	--	$1.15 \times 10^{-6}$
Propylene carbonate	108-32-7	0.08	-0.41	$2.58 \times 10^5$	$3.63 \times 10^{-4}$	--	$3.45 \times 10^{-8}$
Propylene pentamer	15220-87-8	6.28	--	0.05601	$3.92 \times 10^{-1}$	$1.09 \times 10^{-3}$	--
p-Xylene	106-42-3	3.09	3.15	228.6	$6.56 \times 10^{-3}$	$6.14 \times 10^{-3}$	$6.90 \times 10^{-3}$
Pyrimidine	289-95-2	-0.06	-0.4	$2.87 \times 10^5$	$2.92 \times 10^{-6}$	--	--
Pyrrole	109-97-7	0.88	0.75	$3.12 \times 10^4$	$9.07 \times 10^{-6}$	$7.73 \times 10^{-6}$	$1.80 \times 10^{-5}$
Quaternary ammonium compounds, di-C8-10-alkyldimethyl, chlorides	68424-95-3	2.69	--	90.87	$2.20 \times 10^{-10}$	--	--
Quinaldine	91-63-4	2.69	2.59	498.5	$7.60 \times 10^{-7}$	$2.13 \times 10^{-6}$	--
Quinoline	91-22-5	2.14	2.03	1,711	$6.88 \times 10^{-7}$	$1.54 \times 10^{-6}$	$1.67 \times 10^{-6}$
Rhodamine B	81-88-9	6.03	--	0.0116	--	--	--

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		Estimated	Measured		Bond method	Group method 25	Measured
Sodium 1-octanesulfonate	5324-84-5	1.06	--	5,864	$9.15 \times 10^{-8}$	--	--
Sodium 2-mercaptobenzothiolate	2492-26-4	2.86	2.42	543.4	$3.63 \times 10^{-8}$	--	--
Sodium acetate	127-09-3	0.09	-0.17	$4.76 \times 10^5$	$5.48 \times 10^{-7}$	$2.94 \times 10^{-7}$	$1.00 \times 10^{-7}$
Sodium benzoate	532-32-1	1.87	1.87	2,493	$1.08 \times 10^{-7}$	$4.55 \times 10^{-8}$	$3.81 \times 10^{-8}$
Sodium bicarbonate	144-55-8	-0.46	--	$8.42 \times 10^5$	$6.05 \times 10^{-9}$	--	--
Sodium bis(tridecyl) sulfobutanedioate	2673-22-5	11.15	--	$7.46 \times 10^{-9}$	$8.51 \times 10^{-11}$	--	--
Sodium C14-16 alpha-olefin sulfonate	68439-57-6	4.36	--	2,651	$4.95 \times 10^{-7}$	--	--
Sodium caprylamphopropionate	68610-44-6	-0.26	--	615.1	$1.19 \times 10^{-9}$	$2.45 \times 10^{-10}$	--
Sodium carbonate	497-19-8	-0.46	--	$8.42 \times 10^5$	$6.05 \times 10^{-9}$	--	--
Sodium chloroacetate	3926-62-3	0.34	0.22	$1.95 \times 10^5$	$1.93 \times 10^{-7}$	$8.88 \times 10^{-8}$	$9.26 \times 10^{-9}$
Sodium decyl sulfate	142-87-0	1.44	--	1,617	$1.04 \times 10^{-7}$	--	--
Sodium D-gluconate	527-07-1	-1.87	--	$1.00 \times 10^6$	$4.74 \times 10^{-13}$	--	--

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Sodium diacetate	126-96-5	0.09	-0.17	$4.76 \times 10^5$	$5.48 \times 10^{-7}$	$2.94 \times 10^{-7}$	$1.00 \times 10^{-7}$
Sodium dichloroisocyanurate	2893-78-9	1.28	--	3,613	$3.22 \times 10^{-12}$	--	--
Sodium dl-lactate	72-17-3	-0.65	-0.72	$1.00 \times 10^6$	$1.13 \times 10^{-7}$	--	$8.13 \times 10^{-8}$
Sodium dodecyl sulfate	151-21-3	2.42	--	163.7	$1.84 \times 10^{-7}$	--	--
Sodium erythorbate (1:1)	6381-77-7	-1.88	-1.85	$1.00 \times 10^6$	$4.07 \times 10^{-8}$	--	--
Sodium ethasulfate	126-92-1	0.38	--	$1.82 \times 10^4$	$5.91 \times 10^{-8}$	--	--
Sodium formate	141-53-7	-0.46	-0.54	$9.55 \times 10^5$	$7.50 \times 10^{-7}$	$5.11 \times 10^{-7}$	$1.67 \times 10^{-7}$
Sodium hydroxymethanesulfonate	870-72-4	-3.85	--	$1.00 \times 10^6$	$4.60 \times 10^{-13}$	--	--
Sodium l-lactate	867-56-1	-0.65	-0.72	$1.00 \times 10^6$	$1.13 \times 10^{-7}$	--	$8.13 \times 10^{-8}$
Sodium maleate (1:x)	18016-19-8	0.05	-0.48	$1.04 \times 10^5$	$1.35 \times 10^{-12}$	$8.48 \times 10^{-14}$	--
Sodium N-methyl-N-oleoyltaurate	137-20-2	4.43	--	0.4748	$1.00 \times 10^{-12}$	--	--
Sodium octyl sulfate	142-31-4	0.46	--	$1.58 \times 10^4$	$5.91 \times 10^{-8}$	--	--

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		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Sodium salicylate	54-21-7	2.24	2.26	3,808	$1.42 \times 10^{-8}$	$5.60 \times 10^{-12}$	$7.34 \times 10^{-9}$
Sodium sesquicarbonate	533-96-0	-0.46	--	$8.42 \times 10^5$	$6.05 \times 10^{-9}$	--	--
Sodium thiocyanate	540-72-7	0.58	--	$4.36 \times 10^4$	$1.46 \times 10^{-4}$	--	--
Sodium trichloroacetate	650-51-1	1.44	1.33	$1.20 \times 10^4$	$2.39 \times 10^{-8}$	--	$1.35 \times 10^{-8}$
Sodium xylenesulfonate	1300-72-7	-0.07	--	$5.89 \times 10^4$	$3.06 \times 10^{-9}$	--	--
Sorbic acid	110-44-1	1.62	1.33	$1.94 \times 10^4$	$5.72 \times 10^{-7}$	$4.99 \times 10^{-8}$	--
Sorbitan sesquioleate	8007-43-0	14.32	--	$2.31 \times 10^{-11}$	$7.55 \times 10^{-12}$	$1.25 \times 10^{-16}$	--
Sorbitan, mono-(9Z)-9-octadecenoate	1338-43-8	5.89	--	0.01914	$1.42 \times 10^{-12}$	$5.87 \times 10^{-20}$	--
Sorbitan, monooctadecanoate	1338-41-6	6.1	--	0.01218	$1.61 \times 10^{-12}$	$2.23 \times 10^{-19}$	--
Sorbitan, tri-(9Z)-9-octadecenoate	26266-58-0	22.56	--	$1.12 \times 10^{-19}$	$4.02 \times 10^{-11}$	$2.68 \times 10^{-13}$	--
Styrene	100-42-5	2.89	2.95	343.7	$2.76 \times 10^{-3}$	$2.81 \times 10^{-3}$	$2.75 \times 10^{-3}$
Sucrose	57-50-1	-4.27	-3.7	$1.00 \times 10^6$	$4.47 \times 10^{-22}$	--	--

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Chemical name	CASRN	Log $K_{ow}$		Water solubility Estimate from log $K_{ow}$ (mg/L at 25°C)	Henry's law constant (atm-m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured		Bond method	Group method 25	Measured
Sulfan blue	129-17-9	-1.34	--	50.67	$1.31 \times 10^{-26}$	--	--
Sulfuric acid, mono-C12-18-alkyl esters, sodium salts	68955-19-1	3.9	--	5.165	$4.29 \times 10^{-7}$	--	--
Sulfuric acid, mono-C6-10-alkyl esters, ammonium salts	68187-17-7	0.46	--	$1.58 \times 10^4$	$5.91 \times 10^{-8}$	--	--
Symclosene	87-90-1	0.94	--	4,610	$6.19 \times 10^{-11}$	--	--
tert-Butyl hydroperoxide	75-91-2	0.94	--	$1.97 \times 10^4$	$1.60 \times 10^{-5}$	--	--
tert-Butyl perbenzoate	614-45-9	2.89	--	159.2	$2.06 \times 10^{-4}$	--	--
Tetradecane	629-59-4	7.22	7.2	0.009192	$1.65 \times 10^1$	$2.68 \times 10^1$	9.20
Tetradecyldimethylbenzylammonium chloride	139-08-2	3.91	--	3.608	$1.34 \times 10^{-11}$	--	--
Tetraethylene glycol	112-60-7	-2.02	--	$1.00 \times 10^6$	$4.91 \times 10^{-13}$	$5.48 \times 10^{-19}$	--
Tetraethylenepentamine	112-57-2	-3.16	--	$1.00 \times 10^6$	$2.79 \times 10^{-20}$	$4.15 \times 10^{-23}$	--

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm-m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Tetrakis(hydroxymethyl)phosphonium sulfate	55566-30-8	-5.03	--	$1.00 \times 10^6$	$9.17 \times 10^{-13}$	--	--
Tetramethylammonium chloride	75-57-0	-4.18	--	$1.00 \times 10^6$	$4.17 \times 10^{-12}$	--	--
Thiamine hydrochloride	67-03-8	0.95	--	3,018	$8.24 \times 10^{-17}$	--	--
Thiocyanic acid, ammonium salt	1762-95-4	0.58	--	$4.36 \times 10^4$	$1.46 \times 10^{-4}$	--	--
Thioglycolic acid	68-11-1	0.03	0.09	$2.56 \times 10^5$	$1.94 \times 10^{-8}$	--	--
Thiourea	62-56-6	-1.31	-1.08	$5.54 \times 10^5$	$1.58 \times 10^{-7}$	--	$1.98 \times 10^{-9}$
Toluene	108-88-3	2.54	2.73	573.1	$5.95 \times 10^{-3}$	$5.73 \times 10^{-3}$	$6.64 \times 10^{-3}$
Tributyl phosphate	126-73-8	3.82	4	7.355	$3.19 \times 10^{-6}$	--	$1.41 \times 10^{-6}$
Tributyltetradecylphosphonium chloride	81741-28-8	11.22	--	$7.90 \times 10^{-7}$	$2.61 \times 10^{-1}$	--	--
Tridecane	629-50-5	6.73	--	0.02746	$1.24 \times 10^1$	$1.90 \times 10^1$	2.88
Triethanolamine	102-71-6	-2.48	-1	$1.00 \times 10^6$	$4.18 \times 10^{-12}$	$3.38 \times 10^{-19}$	$7.05 \times 10^{-13}$

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm-m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Triethanolamine hydrochloride	637-39-8	-2.48	-1	$1.00 \times 10^6$	$4.18 \times 10^{-12}$	$3.38 \times 10^{-19}$	$7.05 \times 10^{-13}$
Triethanolamine hydroxyacetate	68299-02-5	-2.97	--	$1.00 \times 10^6$	$6.28 \times 10^{-11}$	--	--
Triethyl citrate	77-93-0	0.33	--	$2.82 \times 10^4$	$6.39 \times 10^{-10}$	--	$3.84 \times 10^{-9}$
Triethyl phosphate	78-40-0	0.87	0.8	$1.12 \times 10^4$	$5.83 \times 10^{-7}$	--	$3.60 \times 10^{-8}$
Triethylene glycol	112-27-6	-1.75	-1.75	$1.00 \times 10^6$	$3.16 \times 10^{-11}$	$2.56 \times 10^{-16}$	--
Triethylenetetramine	112-24-3	-2.65	--	$1.00 \times 10^6$	$9.30 \times 10^{-17}$	$6.74 \times 10^{-19}$	--
Triisopropanolamine	122-20-3	-1.22	--	$1.00 \times 10^6$	$9.77 \times 10^{-12}$	$4.35 \times 10^{-18}$	--
Trimethanolamine	14002-32-5	-3.95	--	$1.00 \times 10^6$	$1.42 \times 10^{-8}$	--	--
Trimethylamine	75-50-3	0.04	0.16	$1.00 \times 10^6$	$3.65 \times 10^{-5}$	$1.28 \times 10^{-4}$	$1.04 \times 10^{-4}$
Tripotassium citrate monohydrate	6100-05-6	-1.67	-1.64	$1.00 \times 10^6$	$8.33 \times 10^{-18}$	--	$4.33 \times 10^{-14}$
Tripropylene glycol monomethyl ether	25498-49-1	-0.2	--	$1.96 \times 10^5$	$2.36 \times 10^{-11}$	$4.55 \times 10^{-13}$	--
Trisodium citrate	68-04-2	-1.67	-1.64	$1.00 \times 10^6$	$8.33 \times 10^{-18}$	--	$4.33 \times 10^{-14}$

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Chemical name	CASRN	Log $K_{ow}$		Water solubility	Henry's law constant (atm-m <sup>3</sup> /mol at 25°C)		
		Estimated	Measured	Estimate from log $K_{ow}$ (mg/L at 25°C)	Bond method	Group method 25	Measured
Trisodium citrate dihydrate	6132-04-3	-1.67	-1.64	$1.00 \times 10^6$	$8.33 \times 10^{-18}$	--	$4.33 \times 10^{-14}$
Trisodium ethylenediaminetetraacetate	150-38-9	-3.86	--	$2.28 \times 10^5$	$1.17 \times 10^{-23}$	--	$5.77 \times 10^{-16}$
Trisodium ethylenediaminetriacetate	19019-43-3	-4.32	--	$1.00 \times 10^6$	$3.58 \times 10^{-20}$	--	--
Tromethamine	77-86-1	-1.56	--	$1.00 \times 10^6$	$8.67 \times 10^{-13}$	--	--
Undecane	1120-21-4	5.74	--	0.2571	7.04	9.52	1.93
Urea	57-13-6	-1.56	-2.11	$4.26 \times 10^5$	$3.65 \times 10^{-10}$	--	$1.74 \times 10^{-12}$
Xylenes	1330-20-7	3.09	3.2	207.2	$6.56 \times 10^{-3}$	$6.14 \times 10^{-3}$	$7.18 \times 10^{-3}$

"--" indicates no information available.

1 The EPI (Estimation Programs Interface) Suite™ ([U.S. EPA, 2012a](#)) is an open-source, Windows®-  
2 based suite of physicochemical property and environmental fate estimation programs developed by  
3 the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation. More  
4 information on EPI Suite™ is available at <http://www.epa.gov/oppt/exposure/pubs/episuite.htm>.

5 Although only physicochemical properties from EPI Suite™ are provided here, other sources of  
6 information were also consulted. QikProp ([Schrodinger, 2012](#)) and LeadScope® ([Inc., 2012](#)) are  
7 commercial products designed primarily as drug development and screening tools. QikProp is  
8 specifically focused on drug discovery and provides predictions for physically significant  
9 descriptors and pharmaceutically (and toxicologically) relevant properties useful in predicting  
10 ADME (adsorption, distribution, metabolism, and excretion) characteristics of drug candidates.  
11 QikProp's use of whole-molecule descriptors that have a straightforward physical interpretation (as  
12 opposed to fragment-based descriptors).

13 LeadScope® is a program designed for interpreting chemical and biological screening data that can  
14 assist pharmaceutical scientists in finding promising drug candidates. The software organizes the  
15 chemical data by structural features familiar to medicinal chemists. Graphs are used to summarize  
16 the data, and structural classes are highlighted that are statistically correlated with biological  
17 activity. It incorporates chemically-based data mining, visualization, and advanced informatics  
18 techniques (e.g., prediction tools, scaffold generators). Note that properties generated by QikProp  
19 and LeadScope® are generally more relevant to drug development than to environmental  
20 assessment.

21 Physicochemical properties of chemicals were generated from the two-dimensional (2-D) chemical  
22 structures from the EPA National Center for Computational Toxicology's Distributed Structure-  
23 Searchable Toxicity (NCCT DSSTox) Database Network in structure-data file (SDF) format. For EPI  
24 Suite™ properties, both the desalted and non-desalted 2-D files were run using the program's batch  
25 mode (i.e., processing many molecules at once) to calculate environmentally-relevant, chemical  
26 property descriptors. The chemical descriptors in QikProp require 3-D chemical structures. For  
27 these calculations, the 2-D desalted chemical structures were converted to 3-D using the Rebuild3D  
28 function in the Molecular Operating Environment software ([CCG, 2011](#)). All computed  
29 physicochemical properties are added into the structure-data file prior to assigning toxicological  
30 properties.

31 Both LeadScope® and Qikprop software require input of desalted structures. Therefore, the  
32 structures were desalted, a process where salts and complexes are simplified to the neutral,  
33 uncomplexed form of the chemical, using "Desalt Batch" option in ACD Labs ChemFolder. All  
34 LeadScope® general chemical descriptors (Parent Molecular Weight, AlogP, Hydrogen Bond  
35 Acceptors, Hydrogen Bond Donors, Lipinski Score, Molecular Weight, Parent Atom Count, Polar  
36 Surface Area, and Rotatable Bonds) were calculated by default.

37 All physicochemical properties generated from EPI Suite™, QikProp, and LeadScope® will be made  
38 available to the public in an electronic format in 2015.

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## Appendix D

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# Designing, Constructing, and Testing Wells for Integrity

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*This document is a draft for review purposes only and does not constitute Agency policy.*

## Appendix D. Designing, Constructing, and Testing Wells for Integrity

1 This appendix presents the goals for the design and construction of oil and gas production wells,  
2 the well components used to achieve those goals, and methods for testing well integrity to help  
3 verify that the goals for well performance are achieved. This information provides additional  
4 background for the well component discussions presented in Chapter 6. Information on the  
5 pathways associated with the well that can cause fluid movement into drinking water resources is  
6 presented in Chapter 6.

### D.1. Design Goals for Well Construction

7 Simply stated, production wells are designed to move oil and gas from the production zone (within  
8 the oil and gas reservoir) into the well and then through the well to the surface. There are typically  
9 a variety of goals for well design ([Renpu, 2011](#)), but the main purposes are facilitating the flow of  
10 oil and gas from the hydrocarbon reservoirs to the well (production management) while isolating  
11 that oil and gas and the hydrocarbon reservoirs from nearby ground water resources (zonal  
12 isolation).

13 To achieve these goals, operators design and construct wells to have and maintain mechanical  
14 integrity throughout the life of the well. A properly designed and constructed well has two types of  
15 mechanical integrity: internal and external. Internal mechanical integrity refers to the absence of  
16 significant leakage within the production tubing, casing, or packer. External mechanical integrity  
17 refers to the absence of significant leakage along the well outside of the casing.

18 Achieving mechanical integrity involves designing the well components to resist the stresses they  
19 will encounter. Each well component must be designed to withstand all of the stresses to which the  
20 well will be subjected, including burst pressure, collapse, tensile, compression (or bending), and  
21 cyclical stresses (see Section 6.2.1 for additional information on these stresses). Well materials  
22 should also be compatible with the fluids (including liquids or gases) with which they come into  
23 contact to prevent leaks caused by corrosion.

24 These goals are accomplished by the use of one or more layers of casing, cement, and mechanical  
25 devices (such as packers), which provide the main barrier preventing migration of fluids from the  
26 well into drinking water sources.

### D.2. Well Components

27 Casing and cement are used in the design and construction of wells to achieve the goals of  
28 mechanical integrity and zonal isolation. Several industry-developed specifications and best  
29 practices for well construction have been established to guide well operators in the construction  
30 process; see Text Box D-1. (Information is not available to determine how often these practices are  
31 used or how well they prevent the development of pathways for fluid movement to drinking water  
32 resources.) The sections below describe options available for casing, cement, and other well  
33 components.

### Text Box D-1. Selected Industry-Developed Specifications and Recommended Practices for Well Construction in North America.

#### 1 *American Petroleum Institute (API)*

- 2 • API Guidance Document HF1—Hydraulic Fracturing Operations—Well Construction and Integrity
- 3 Guidelines ([API, 2009a](#))
- 4 • API RP 10B-2—Recommended Practice for Testing Well Cements ([API, 2013](#))
- 5 • API RP 10D-2—Recommended Practice for Centralizer Placement and Stop Collar Testing ([API, 2004](#))
- 6 • API RP 5C1—Recommended Practices for Care and Use of Casing and Tubing ([API, 1999](#))
- 7 • API RP 65-2—Isolating Potential Flow Zones during Well Construction ([API, 2010a](#))
- 8 • API Specification 10A—Specification on Cements and Materials for Well Cementing ([API, 2010b](#))
- 9 • API Specification 11D1—Packers and Bridge Plugs ([API, 2009b](#))
- 10 • API Specification 5CT—Specification for Casing and Tubing ([API, 2011](#))

#### 11 *Canadian Association of Petroleum Producers (CAPP) and Enform*

- 12 • Hydraulic Fracturing Operating Practices: Wellbore Construction and Quality Assurance ([CAPP, 2013](#))
- 13 • Interim Industry Recommended Practice Volume #24—Fracture Stimulation: Inter-wellbore
- 14 Communication ([Enform, 2013](#))

#### 15 *Marcellus Shale Coalition (MSC)*

- 16 • Recommended Practices—Drilling and Completions ([MSC, 2013](#))

### D.2.1. Casing

17 Casing is steel pipe that is placed into the wellbore (the cylindrical hole drilled through the  
18 subsurface rock formation) to maintain the stability of the wellbore, to transport the hydrocarbons  
19 from the subsurface to the surface, and to prevent intrusion of other fluids into the well and  
20 wellbore. Up to four types of casing may be present in a well, including (from largest to smallest-  
21 diameter): conductor casing, surface casing, intermediate casing, and production casing. Each is  
22 described below.

23 The **conductor casing** is the largest diameter string of casing. It is typically in the range of 30 in.  
24 (76 cm) to 42 in. (107 cm) in diameter ([Hyne, 2012](#)). Its main purpose is to prevent unconsolidated  
25 material, such as sand, gravel, and soil, from collapsing into the wellbore. Therefore, the casing is  
26 typically installed from the surface to the top of the bedrock or other consolidated formations. The  
27 conductor casing may or may not be cemented in place.

28 The next string of casing is the **surface casing**. A typical surface casing diameter is 13.75 in. (34.93  
29 cm), but diameter can vary ([Hyne, 2012](#)). The surface casing's main purposes are to isolate any  
30 ground water resources that are to be protected by preventing fluid migration along the wellbore

1 once the casing is cemented and to provide a sturdy structure to which blow-out prevention  
2 equipment can be attached. For these reasons, the surface casing most commonly extends from the  
3 surface to some distance beneath the lowermost geologic formation containing ground water  
4 resources to be protected. The specific depth to which the surface casing is set is often governed by  
5 the depth of the ground water resource as defined and identified for protection in state regulations.

6 **Intermediate casing** is typically used in wells to control pressure in an intermediate-depth  
7 formation. It may be used to reduce or prevent exposure of weak formations to pressure from the  
8 weight of the drilling fluid or cement or to allow better control of over-pressured formations. The  
9 intermediate casing extends from the surface through the formation of concern. There may be more  
10 than one string of concentric intermediate casing present or none at all, depending on the  
11 subsurface geology. Intermediate casing may be cemented, especially through over-pressured  
12 zones; however, it is not always cemented to the surface. Intermediate casing, when present, is  
13 often 8.625 in. (21.908 cm) in diameter but can vary ([Hyne, 2012](#)).

14 **Production casing** extends from the surface into the production zone. The main purposes of the  
15 production casing are to isolate the hydrocarbon product from fluids in surrounding formations  
16 and to transport the product to the surface. It can also be used to inject fracturing fluids, receive  
17 flowback during hydraulic fracturing operations (e.g., if tubing or a temporary fracturing string is  
18 not present), and prevent other fluids from mixing with and diluting the produced hydrocarbons.  
19 The production casing is generally cemented to some point above the production zone. Production  
20 casing is often 5.5 in. (14.0 cm) in diameter but can vary ([Hyne, 2012](#)).

21 **Liners** are another type of metal tubular (casing-like) well component that can be used to fulfill the  
22 same purposes as intermediate and production casing in the production zone. Like casing, they are  
23 steel pipe, but differ in that they do not extend from the production zone to the surface. Rather, they  
24 are connected to the next largest string of casing by a hanger that is attached to the casing. A frac  
25 sleeve is a specialized type of liner that is used during fracturing. It has plugs that can be opened  
26 and closed by dropping balls from the surface (see the discussion of well completions below for  
27 additional information on the use of frac sleeves).

28 **Production tubing** is the smallest, innermost steel pipe in the well and is distinguished from casing  
29 by not being cemented in place. It is used to transport the hydrocarbons to the surface. Fracturing  
30 may be done through the tubing if present, or through the production casing. Because casing cannot  
31 be replaced, tubing is often used, especially if the hydrocarbons contain corrosive substances such  
32 as hydrogen sulfide or carbon dioxide. Tubing may not be used in high-volume production wells.  
33 Typical tubing diameter is between 1.25 in. (3.18 cm) and 4.5 in. (11.4 cm) ([Hyne, 2012](#)).

### D.2.2. Cement

34 Cement is the main barrier preventing fluid movement along the wellbore outside the casing. It also  
35 lends mechanical strength to the well and protects the casing from corrosion by naturally occurring  
36 formation fluids. Cement is placed in the annulus, which is the space between two adjacent casings  
37 or the space between the outermost casing and the rock formation through which the wellbore was

1 drilled. The sections below describe considerations for selecting cement and additives, as well as  
2 cementing procedures and techniques.

### **D.2.2.1. Considerations for Cementing**

3 The length and location of the casing section to be cemented and the composition of the cement can  
4 vary based on numerous factors, including the presence and locations of weak formations, over- or  
5 under-pressured formations, or formations containing fluids; formation permeability; and  
6 temperature. State requirements for oil and gas production well construction and the relative costs  
7 of well construction options are also factors.

8 Improper cementing can lead to the formation of channels (small connected voids) in the cement,  
9 which can—if they extend across multiple formations or connect to other existing channels or  
10 fractures—present pathways for fluid migration. This section describes some of the considerations  
11 and concerns for proper cement placement and techniques and materials that are available to  
12 address these concerns. Careful selection of cements (and additives) and design of the cementing  
13 job can avoid integrity problems related to cement.

14 To select the appropriate cement type, properties, and additives, operators consider the required  
15 strength needed to withstand downhole conditions and compatibility with subsurface chemistry, as  
16 described below:

- 17 • The cement design needs to **achieve the strength** required under the measured or  
18 anticipated downhole conditions. Factors that are taken into account to achieve proper  
19 strength can include density, thickening time, the presence of free water, compressive  
20 strength, and formation permeability ([Renpu, 2011](#)). Commonly, cement properties are  
21 varied during the process, with a “weaker” (i.e., less dense) lead cement, followed by a  
22 “stronger” (denser) tail cement. The lead cement is designed with a lower density to  
23 reduce pressure on the formation and better displace drilling fluid without a large concern  
24 for strength. The stronger tail cement provides greater strength for the deeper portions of  
25 the well the operator considers as requiring greater strength.
- 26 • The **compatibility of the cement** with the chemistry of formation fluids, hydrocarbons,  
27 and hydraulic fracturing fluids is important for maintaining well integrity through the life  
28 of the well. Most oil and gas wells are constructed using some form of Portland cement.  
29 Portland cement is a specific type of cement consisting primarily of calcium silicates with  
30 additional iron and aluminum. Industry specifications for recommended cements are  
31 determined by the downhole pressure, temperature, and chemical compatibility required.

32 There are a number of considerations in the design and execution of a cement job. Proper  
33 centralization of the casing within the wellbore is one of the more important considerations. Others  
34 include the potential for lost cement, gas invasion, cement shrinkage, incomplete removal of drilling  
35 mud, settling of solids in the wellbore, and water loss into the formation while curing. These  
36 concerns, and techniques available to address them, include the following:

- 1       • **Improper centralization of the casing within the wellbore** can lead to preferential flow  
2 of cement on the side of the casing with the larger space and little to no cement on the side  
3 closest to the formation. If the casing is not centered in the wellbore, cement will flow  
4 unevenly during the cement job, leading to the formation of cement channels. [Kirksey](#)  
5 [\(2013\)](#) notes that, if the casing is off-center by just 25%, the cement job is almost always  
6 inadequate. Centralizers are used to keep the casing in the center of the hole and allow an  
7 even cement job. To ensure proper centralization, centralizers are placed at regular  
8 intervals along the casing ([API, 2010a](#)). Centralizer use is especially key in horizontal  
9 wells, as the casing will tend to settle (due to gravity) to the bottom of the wellbore if the  
10 casing is not centered ([Sabins, 1990](#)), leading to inadequate cement on the lower side.
- 11       • **Lost cement** (sometimes referred to as lost returns) refers to cement that moves out of  
12 the wellbore and into the formation instead of filling up the annulus between the casing  
13 and the formation. Lost cement can occur in weak formations that fail (fracture) under  
14 pressure of the cement or in particularly porous, permeable, or naturally fractured  
15 formations. Lost cement can result in lack of adequate cement across a water- or brine-  
16 bearing zone. To avoid inadequate placement of cement due to lost cement, records of  
17 nearby wells can be examined to determine zones where lost cement returns occur ([API,](#)  
18 [2009a](#)). If records from nearby wells are not available, cores and logs may be used to  
19 identify any high-permeability or mechanically weak formations that might lead to lost  
20 cement. Steps can then be taken to eliminate or reduce loss of cement to the formation.  
21 Staged cementing (see below) can reduce the hydrostatic pressure on the formation and  
22 may avoid fracturing weak formations ([Lyons and Pligsa, 2004](#)). Additives are also  
23 available that will lessen the flow of cement into highly porous formations ([API, 2010a;](#) [Ali](#)  
24 [et al., 2009](#)).
- 25       • **Gas invasion and cement shrinkage** during cement setting can also cause channels and  
26 poor bonding. During the cementing process, the hydrostatic pressure from the cement  
27 column keeps formation gas from entering the cement. As the cement sets (hardens), the  
28 hydrostatic pressure decreases; if it becomes less than the formation pressure, gas can  
29 enter the cement, leading to channels. Cement also shrinks as it sets, which can lead to  
30 poor bonding and formation of microannuli. These problems can be avoided by using  
31 cement additives that increase setting time or expand to offset shrinkage ([McDaniel et al.,](#)  
32 [2014;](#) [Wojtanowicz, 2008;](#) [Dusseault et al., 2000](#)). Foamed cement can help alleviate  
33 problems with shrinkage, although care needs to be taken in cement design to ensure the  
34 proper balance of pressure between the cement column and formation ([API, 2010a](#)).  
35 Cement additives are also available that will expand upon contact with certain fluids such  
36 as hydrocarbons. These cements, termed self-healing cements, are relatively new but have  
37 shown early promise in some fields ([Ali et al., 2009](#)). Rotating the casing during cementing  
38 will also delay cement setting. Another technique called pulsation, where pressure pulses  
39 are applied to the cement while it is setting, also can delay cement setting and loss of  
40 hydrostatic pressure until the cement is strong enough to resist gas penetration ([Stein et](#)  
41 [al., 2003](#)).

- 1 • Another important issue is **removal of drilling mud**. If drilling mud is not completely  
2 removed, it can gather on one side of the wellbore and prevent that portion of the  
3 wellbore from being adequately cemented. The drilling mud can then be eroded away after  
4 the cement sets, leaving a channel. Drilling mud can be removed by circulating a denser  
5 fluid (spacer fluid) to flush the drilling mud out ([Kirksey, 2013](#); [Brufatto et al., 2003](#)).  
6 Mechanical devices called scratchers can also be attached to the casing and the casing  
7 rotated or reciprocated to scrape drilling mud from the wellbore ([Hyne, 2012](#); [Crook,](#)  
8 [2008](#)). The spacer fluid, which is circulated prior to the cement to wash the drilling fluid  
9 out of the wellbore, must be designed with the appropriate properties and pumped in such  
10 a way that it displaces the drilling fluid without mixing with the cement ([Kirksey, 2013](#);  
11 [API, 2010a](#); [Brufatto et al., 2003](#)).
- 12 • Also of concern in horizontal wells is the possibility of **solids settling** at the bottom of the  
13 wellbore and free water collecting at the top of the wellbore. This can lead to channels and  
14 poor cement bonding. The cement slurry must be properly designed for horizontal wells to  
15 minimize free water and solids settling.
- 16 • If there is free water in the cement, pressure can cause **water loss into the formation**,  
17 leaving behind poor cement or channels ([Jiang et al., 2012](#)). In horizontal wells, free water  
18 can also accumulate at the top of the wellbore, forming a channel ([Sabins, 1990](#)).  
19 Minimizing free water in the cement design and using fluid loss control additives can help  
20 control loss of water ([Ross and King, 2007](#)).

#### D.2.2.2. Cement Placement Techniques

21 The primary cement job is most commonly conducted by pumping the cement down the inside of  
22 the casing, then out the bottom of the casing where it is then forced up the space between the  
23 outside of the casing and the formation. (The cement can also be placed in the space between two  
24 casings.) If **continuous cement** (i.e., a sheath of cement placed along the entire wellbore) is  
25 desired, cement is circulated through the annulus until cement that is pumped down the central  
26 casing flows out of the annulus at the surface. A spacer fluid is often pumped ahead of cement to  
27 remove any excess drilling fluid left in the wellbore; even if the operator does not plan to circulate  
28 cement to the surface, the spacer fluid will still return to the surface, as this is necessary to remove  
29 the drilling mud from the annulus. If neither the spacer fluid nor the cement returns to the surface,  
30 this indicates that fluids are being lost into the formation.

31 **Staged cementing** is a technique that reduces pressure on the formation by decreasing the height  
32 (and therefore the weight) of the cement column. This may be necessary if the estimated weight  
33 and pressure associated with standard cement emplacement could damage zones where the  
34 formation intersected is weak. The reduced hydrostatic pressure at the bottom of the cement  
35 column can also reduce the loss of water to permeable formations, improving the quality of the  
36 cement job. In multiple-stage cementing, cement is circulated to just below a cement collar placed  
37 between two sections of casing. A cement collar will have been placed between two sections of  
38 casing, just above, with ports that can be opened by dropping a weighted tool. Two plugs—which  
39 are often referred to as bombs or darts because of their shape—are then dropped. The first plug is

1 dropped, once the desired cement for the first stage has been pushed out of the casing by a spacer  
2 fluid. It closes the section of the well below the cement collar and stops cement from flowing into  
3 the lower portion of the well. The second plug (or opening bomb) opens the cement ports in the  
4 collar, allowing cement to flow into the annulus between the casing and formation. Cement is then  
5 circulated down the wellbore, out the cement ports, into the annulus, and up to the surface. Once  
6 cementing is complete, a third plug is dropped to close the cement ports, preventing the newly  
7 pumped cement from flowing back into the well ([Lyons and Pligsa, 2004](#)); see Figure D-1.

8 Another less commonly used primary cementing technique is **reverse circulation cementing**. This  
9 technique has been developed to decrease the force exerted on weak formations. In reverse  
10 circulation cementing, the cement is pumped down the annulus directly between the outside of the  
11 outermost casing and the formation. This essentially allows use of lower density cement and lower  
12 pumping pressures. With reverse circulation cementing, greater care must be taken in calculating  
13 the required cement, ensuring proper cement circulation, and locating the beginning and end of the  
14 cemented portion.

15 Another method used to cement specific portions of the well without circulating cement along the  
16 entire wellbore length is to use a **cement basket**. A cement basket is a device that attaches to the  
17 well casing. It is made of flexible material such as canvas or rubber that can conform to the shape of  
18 the wellbore. The cement basket acts as a one-way barrier to cement flow. Cement can be circulated  
19 up the wellbore past the cement basket, but when circulation stops the basket prevents the cement  
20 from falling back down the wellbore. Cement baskets can be used to isolate weak formations or  
21 formations with voids. They can also be placed above large voids such as mines or caverns with  
22 staged cementing used to cement the casing above the void.

23 If any deficiencies are identified, **remedial cementing** may be performed. The techniques available  
24 to address deficiencies in the primary cement job including cement squeezes or top-job cementing.  
25 A cement squeeze injects cement under high pressure to fill in voids or spaces in the primary  
26 cement job caused by high pressure, failed formations, or improper removal of drilling mud.  
27 Although cement squeezes can be used to fix deficiencies in the primary cement job, they require  
28 the well to be perforated, which can weaken the well and make it susceptible to degradation by  
29 pressure and temperature cycling as would occur during fracturing ([Crescent, 2011](#)). Another  
30 method of secondary cementing is the top job. In a top job, cement is pumped down the annulus  
31 directly to fill the remaining uncemented space when cement fails to circulate to the surface.

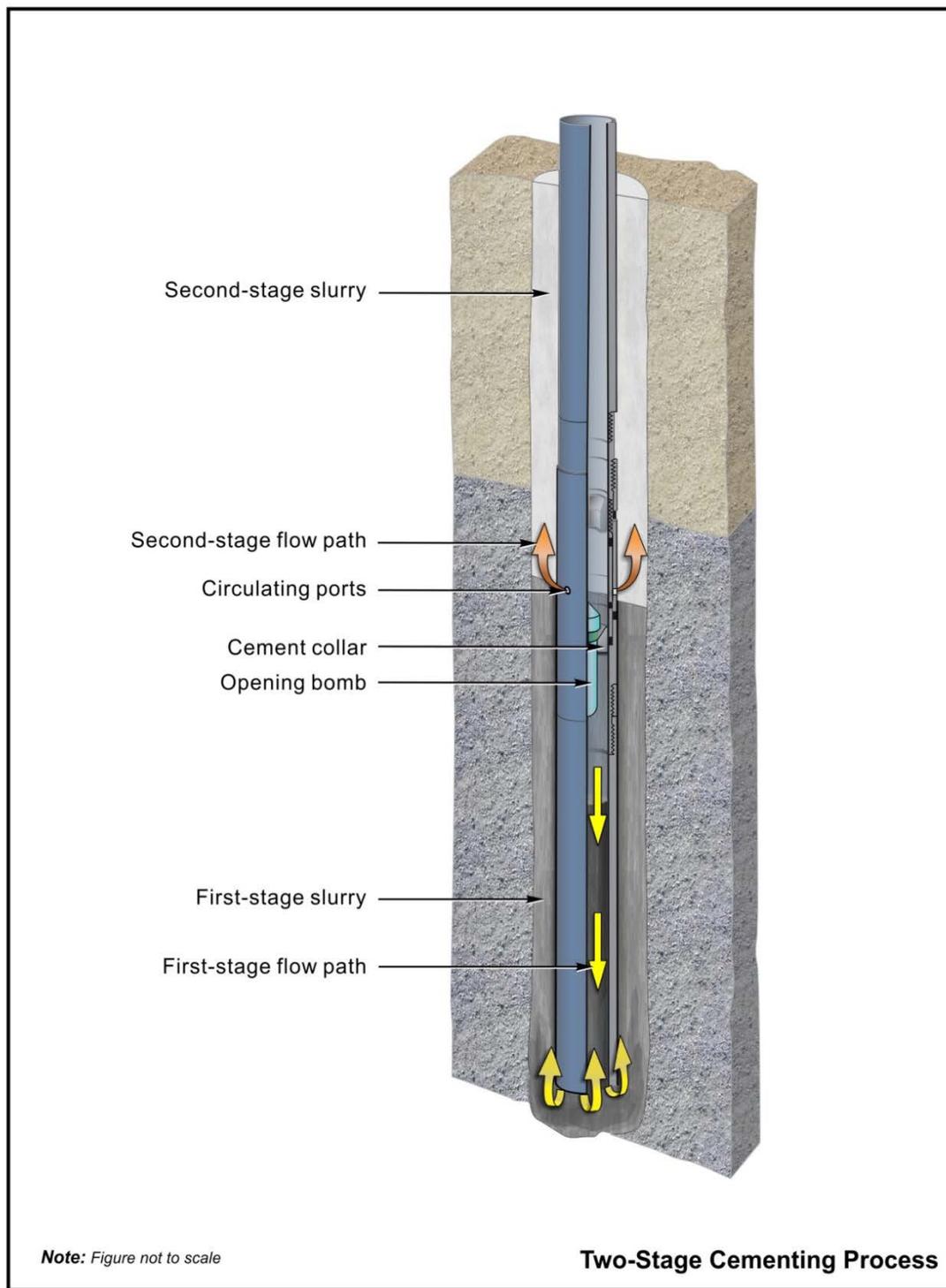
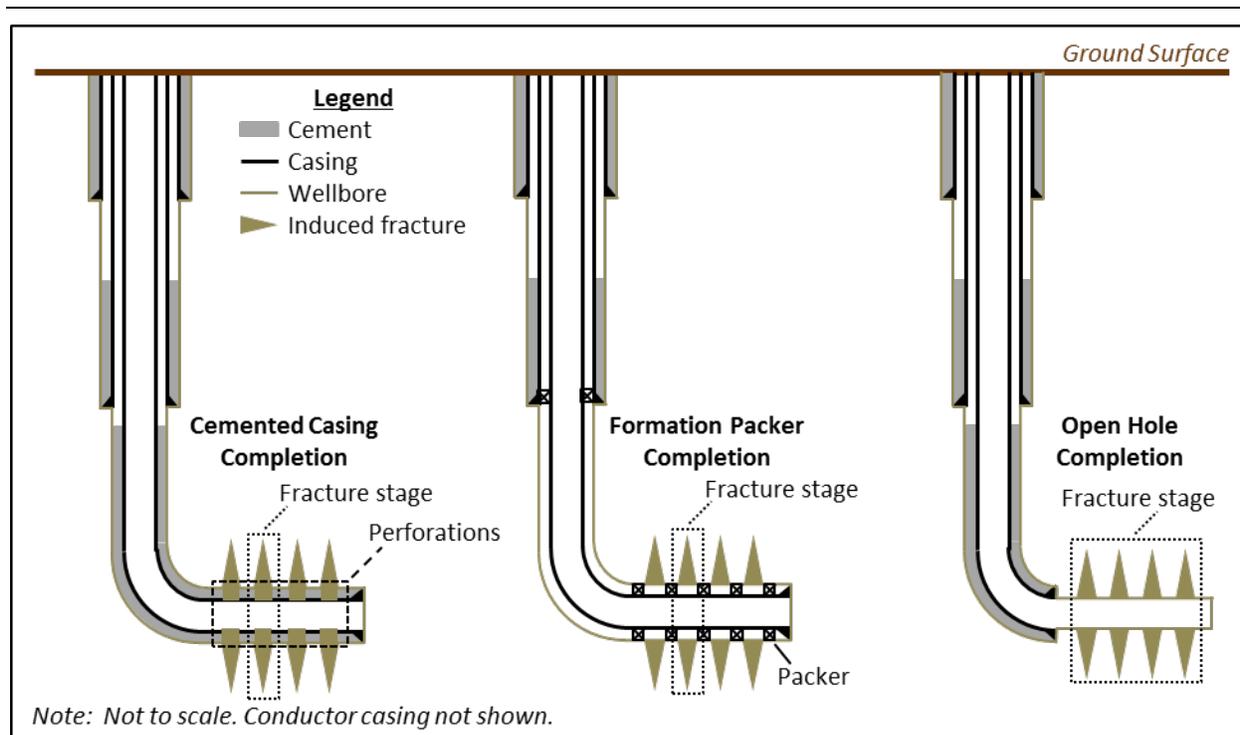


Figure D-1. A typical staged cementing process.

### D.3. Well Completions

- 1 Completion refers to how the well is prepared for production and how flow is established between
- 2 the formation and the surface. Figure D-2 presents examples of well completion types, including
- 3 cased, formation packer, and open hole completion.



**Figure D-2. Examples of well completion types.**

Configurations shown include cased, formation packer, and open hole completion. From [U.S. EPA \(2015f\)](#).

- 4 A **cased completion**, where the casing extends to the end of the wellbore and is cemented in place,
- 5 is the most common configuration of the well in the production zone ([U.S. EPA, 2015f](#)). Perforations
- 6 are made through the casing and cement and into the formation using small explosive charges
- 7 called “perf guns” or other devices, such as sand jets. Hydraulic fracturing then is conducted
- 8 through the perforations. This is a common technique in wells that produce from several different
- 9 depths and in low-permeability formations that are fractured ([Renpu, 2011](#)). While perforations do
- 10 control the initiation point of the fracture, this can be a disadvantage if the perforations are not
- 11 properly aligned with the local stress field. If the perforations are not aligned, the fractures will
- 12 twist to align with the stress field, leading to tortuosity in the fractures and making fluid movement
- 13 through them more difficult ([Cramer, 2008](#)). Fracturing stages can be isolated from each other
- 14 using various mechanisms such as plugs or baffle rings, which close off a section of the well when a
- 15 ball of the correct size is dropped down the well.

1 **A packer** is a mechanical device used to selectively seal off certain sections of the wellbore.  
2 Packers can be used to seal the space between the tubing and casing, between two casings, or  
3 between the production casing and formation. The packer has one or more rubber elements that  
4 can be manipulated downhole to increase in diameter and make contact with the inner wall of the  
5 next-largest casing or the formation, effectively sealing the annulus created between the outside of  
6 the tubing and the inside of the casing. Packers vary in how they are constructed and how they are  
7 set, based on the downhole conditions in which they are used. There are two types of packers:  
8 internal packers and formation packers. Internal packers are used to seal the space between the  
9 casing and tubing or between two different casings. They isolate the outer casing layers from  
10 produced fluids and prevent fluid movement into the annulus. Formation packers seal the space  
11 between the casing and the formation and are often used to isolate fracture stages; they can be used  
12 to separate an open hole completion into separate fracture stages. Packers can seal an annulus by  
13 several different mechanisms. Mechanical packers expand mechanically against the formation and  
14 can exert a significant force on the formation. Swellable packers have elastomer sealing elements  
15 that swell when they come into contact with a triggering fluid such as water or hydrocarbons. They  
16 exert less force on the formation and can seal larger spaces but take some time to fully swell  
17 ([McDaniel and Rispler, 2009](#)). Internal mechanical integrity tests such as pressure tests can verify  
18 that the packer is functioning as designed and has not corroded or deteriorated.

19 In an **open hole completion**, the production casing extends just into the production zone and the  
20 entire length of the wellbore through the production zone is left uncased. This is only an option in  
21 formations where the wellbore is stable enough to not collapse into the wellbore. In formations that  
22 are unstable, a slotted liner may be used in open hole completions to control sand production  
23 ([Renpu, 2011](#)). Perforations are not needed in an open hole completion, since the production zone  
24 is not cased. An open hole completion can be fractured in a single stage or in multiple stages.

25 If formations are to be fractured in stages, additional completion methods are needed to separate  
26 the stages from each other and control the location of the fractures. One possibility is use of a liner  
27 with formation packers to isolate each stage. The liner is equipped with sliding sleeves that can be  
28 opened by dropping balls down the casing to open each stage. Fracturing typically occurs from the  
29 end of the well and continues toward the beginning of the production zone.

#### D.4. Mechanical Integrity Testing

30 While proper design and construction of the well's casing and cement are important, it is also  
31 important to verify the well was constructed and is performing as designed. Mechanical integrity  
32 tests (MITs) can verify that the well was constructed as planned and can detect damage to the  
33 production well that occurs during operations, including hydraulic fracturing activities. Verifying  
34 that a well has mechanical integrity can prevent potential impacts to drinking water resources by  
35 providing early warning of a problem with the well or cement and allowing repairs.

36 It is important to note that if a well fails an MIT, this does not mean the well has failed or that an  
37 impact on drinking water resources has occurred. An MIT failure is a warning that one or more  
38 components of the well are not performing as designed and is an indication that corrective actions

1 are necessary. If well remediation is not performed, a loss of well integrity could occur, which could  
2 result in fluid movement from the well.

#### D.4.1. Internal Mechanical Integrity

3 Internal mechanical integrity is an absence of significant leakage in the tubing, casing, or packers  
4 within the well system. Loss of internal mechanical integrity is usually due to corrosion or  
5 mechanical failure of the well's tubular and mechanical components.

6 Internal mechanical integrity can be tested by the use of pressure testing, annulus pressure  
7 monitoring, ultrasonic monitoring, and casing inspection logs or caliper logs:

- 8 • **Pressure testing** involves raising the pressure in the wellbore to a set level and shutting  
9 in the well. If the well has internal mechanical integrity, the pressure should remain  
10 constant with only small changes due to temperature fluctuation. Typically, the well is  
11 shut in (i.e., production is stopped and the wellhead valves closed) for half an hour, and if  
12 the pressure remains within 5% of the original reading, the well is considered to have  
13 passed the test. Usually, the well is pressure tested to the maximum expected pressure; for  
14 a well to be used for hydraulic fracturing this would be the pressure applied during  
15 hydraulic fracturing. Pressure tests, however, can cause debonding of the cement from the  
16 casing, so test length is often limited to reduce this effect ([API, 2010a](#)).
- 17 • If the annulus between the tubing and casing is sealed by a packer, **annulus pressure**  
18 **monitoring** can give an indication of the integrity of the tubing and casing. If the tubing,  
19 casing, and packer all have mechanical integrity, the pressure in the annulus should not  
20 change except for small changes in response to temperature fluctuations. The annulus can  
21 be filled with a non-corrosive liquid and the level of the liquid can be used as another  
22 indication of the integrity of the casing, tubing, and packer. The advantage of monitoring  
23 the tubing/production casing annulus is it can give a continuous, real-time indication of  
24 the internal integrity of the well. Even if the annulus is not filled with a fluid, monitoring its  
25 pressure can indicate leaks. If pressure builds up in the annulus and then recovers quickly  
26 after having bled off, that condition is referred to as sustained casing pressure or surface  
27 casing vent flow and is a sign of a leak in the tubing or casing ([Watson and Bachu, 2009](#)).  
28 Monitoring of annuli between other sets of casings can also provide information on the  
29 integrity of those casings. It can also provide information on external mechanical integrity  
30 for annuli open to the formation (see Section D.4.2 for additional information on external  
31 MITs). [Jackson et al. \(2013\)](#) also note that monitoring annular pressure allows the  
32 operator to vent gas before it accumulates enough pressure to cause migration into  
33 drinking water resources. Measuring annulus flow rate also allows detection of gas  
34 flowing into the annulus ([Arthur, 2012](#)).
- 35 • A newer tool uses **ultrasonic monitors** to detect leaks in casing and other equipment. It  
36 measures the attenuation of an ultrasonic signal as it is transmitted through the wellbore.  
37 The tool measures transmitted ultrasonic signals as it is lowered down the wellbore. The  
38 tool can pick up ultrasonic signals created by the leak, similar to noise logs. The tool only

1 has a range of a few feet but is claimed to detect leaks as small as half a cup per minute  
2 ([Julian et al., 2007](#)).

- 3 • **Caliper logs** have mechanical fingers that extend from a central tool and measure the  
4 distance from the center of the wellbore to the side of the casing. Running a caliper log can  
5 identify areas where corrosion has altered the diameter of the casing or where holes have  
6 formed in the casing. Caliper logs may also detect debris or obstructions in the well. Casing  
7 inspection and caliper logs are primarily used to determine the condition of the casing.  
8 Regular use of them may identify problems such as corrosion and allow mitigation before  
9 they cause of loss of integrity to the casing. To run these logs in a producing well, the  
10 tubing must first be pulled.
- 11 • **Casing inspection logs** are instruments lowered into the casing to inspect the casing for  
12 signs of wear or corrosion. One type of casing log uses video equipment to detect  
13 corrosion or holes. Another type uses electromagnetic pulses to detect variations in metal  
14 thickness. Running these logs in a producing well requires the tubing to be pulled.

15 If an internal mechanical integrity problem is detected, first, the location of the problem must be  
16 found. Caliper or casing inspection logs can detect locations of holes in casing. Locations of leaks  
17 can also be detected by sealing off different sections of the well using packers and performing  
18 pressure tests on each section until the faulty section is located. If the leaks are in the tubing or a  
19 packer, the problem may be remedied by replacing the well component. Casing leaks may be  
20 remedied by performing a cement squeeze (see the section on cementing).

#### D.4.2. External Mechanical Integrity

21 External well mechanical integrity is demonstrated by establishing the absence of significant fluid  
22 movement along the outside of the casing, either between the outer casing and cement or between  
23 the cement and the wellbore. Failure of an external MIT can indicate improper cementing or  
24 degradation of the cement emplaced in the annular space between the outside of the casing and the  
25 wellbore. This type of failure can lead to movement of fluids out of intended production zones and  
26 toward drinking water resources.

27 Several types of logs are available to evaluate external mechanical integrity, including temperature  
28 logs, noise logs, oxygen activation logs, radioactive tracer logs, and cement evaluation logs.

- 29 • **Temperature logs** measure the temperature in the wellbore. They are capable of  
30 measuring small changes in temperature. They can be performed using instruments that  
31 are lowered down the well on a wireline or they can be done using fiber optic sensors  
32 permanently installed in the well. When performed immediately after cementing, they can  
33 detect the heat from the cement setting and determine the location of the top of cement.  
34 After the cement has set, temperature logs can sense the difference in temperatures  
35 between formation fluids and injected or produced fluids. They may also detect  
36 temperature changes due to cooling or warming caused by flow. In this way temperature  
37 logs may detect movement of fluid outside the casing in the wellbore ([Arthur, 2012](#)).

1 Temperature logs require interpretation of the causes of temperature changes and are  
2 therefore subject to varying results among different users.

- 3 • **Noise logs** are sensitive microphones that are lowered down the well on a wireline. They  
4 are capable of detecting small noises caused by flowing fluids, such as fluids flowing  
5 through channels in the cement ([Arthur, 2012](#)). They are most effective at detecting fast-  
6 moving gas leaks and less successful with more slowly moving liquid migration.
- 7 • **Oxygen activation logs** consist of a neutron source and one or more detectors that are  
8 lowered on a wireline. The neutron source bombards oxygen molecules surrounding the  
9 wellbore and converts them into unstable nitrogen molecules that rapidly decay back to  
10 oxygen, emitting gamma radiation in the process. Gamma radiation detectors above or  
11 below the neutron source measure how quickly the oxygen molecules are moving away  
12 from the source, thereby determining flow associated with water.
- 13 • **Radioactive tracer logs** involve release of a radioactive tracer and then passing a  
14 detector up or down the wellbore to measure the path the tracers have taken. They can be  
15 used to determine if fluid is flowing up the wellbore. Tracer logs can be very sensitive but  
16 may be limited in the range over which leaks can be detected.
- 17 • **Cement evaluation logs** (also known as cement bond logs) are acoustic logs consisting of  
18 an instrument that sends out acoustic signals along with receivers, separated by some  
19 distance, that record the acoustic signals. As the acoustic signals pass through the casing  
20 they will be attenuated to an extent, depending on whether the pipe is free or is bonded to  
21 cement. By analyzing the return acoustic signal, the degree of cement bonding with the  
22 casing can be determined. The cement evaluation log measures the sound attenuation as  
23 sound waves passing through the cement and casing. There are different types of cement  
24 evaluation logs available. Some instruments can only return an average value over the  
25 entire wellbore. Other instruments are capable of measuring the cement bond radially.  
26 Cement logs do not actually determine whether fluid movement through the annulus is  
27 occurring. They only can determine whether cement is present in the annulus and in some  
28 cases can give a qualitative assessment of the quality of the cement in the annulus. Cement  
29 evaluation logs are used to calculate a bond index which varies between 0 and 1, with 1  
30 representing the strongest bond and 0 representing the weakest bond.

31 If the well fails an external MIT, damaged or missing cement may be repaired using a cement  
32 squeeze ([Wojtanowicz, 2008](#)). A cement squeeze involves injection of cement slurry into voids  
33 behind the casing or into permeable formations. Different types of cement squeezes are available  
34 depending on the location of the void needing to be filled and well conditions ([Kirksey, 2013](#)).  
35 Cement squeezes are not always successful, however, and may need to be repeated to successfully  
36 seal off flow ([Wojtanowicz, 2008](#)).

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## Appendix E

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# Flowback and Produced Water Supplemental Tables and Information

## Appendix E. Flowback and Produced Water Supplemental Tables and Information

### E.1. Flowback and Long-Term Produced Water Volumes

- 1 The EPA ([2015g](#)) estimates of flowback volumes and long-term produced water volumes used to
- 2 generate the summaries appearing in Table 7-3 of Chapter 7 appear below in Table E-1.

**Table E-1. Flowback and long-term produced water characteristics for wells in unconventional formations, formation-level data.**

Source: [U.S. EPA \(2015g\)](#).

Basin	Resource Type	Unconventional Formation	Drill Type	Fracturing Fluid (Mgal)			Flowback (% of Fracturing Fluid Returned)			Long-Term Produced Water Rates (gpd)		
				Median	Range	Number of Data Points	Median	Range <sup>a</sup>	Number of Data Points	Median	Range <sup>b</sup>	Number of Data Points
Anadarko	Shale	Woodford	H	4.7	1.0-12	2,239	34	20-50	3	5,500	3,200-6,400	198
	Tight	Cleveland	H	0.81	0.2-4.0	144	--	12-40	2	82	20-300	571
			V	0.69	0.11-3	4	--	--	2	32	6.6-170	390
		Granite Wash	H	6.2	0.2-9.4	77	--	7-22	2	1,300	0-2,200	273
			V	0.56	0.05-3	26	--	--	2	500	170-1,300	2,413
		Mississippi Lime	H	1.8	0.82-2.4	428	--	50	1	--	37,000-120,000	4
Appalachian	Shale	Marcellus	H	4.4	0.9-11	14,010	7	4-47	4,374	860	54-13,000	4,984
			V	2.6	0.53-6.6	66	40	21-60	7	230	100-1,200	714
		Utica	H	4.0	1.0-11	150	4	2-27	73	510	210-1,200	82
Arkoma	Shale	Fayetteville	H	5.1	1.7-11	1,668	--	10-20	2	430	150-2,300	2,305
Denver-Julesburg	Shale	Niobrara	H	2.6	0.73-3.4	69	13	6-25	16	680	260-810	250
			V	0.32	0.27-3.3	367	11	7-35	9	340	240-600	5,474
	Tight	Codell	D	0.28	0.21-0.46	78	--	--	0	--	--	0
			V	0.27	0.13-0.46	185	--	--	0	--	--	0
		Codell-Niobrara	H	2.6	0.15-2.7	62	7	--	32	34	19-140	32
	D		0.45	0.21-0.47	116	--	--	0	--	--	0	
	V		0.30	0.13-0.46	592	--	--	0	29	13-65	1,677	

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Basin	Resource Type	Unconventional Formation	Drill Type	Fracturing Fluid (Mgal)			Flowback (% of Fracturing Fluid Returned)			Long-Term Produced Water Rates (gpd)		
				Median	Range	Number of Data Points	Median	Range <sup>a</sup>	Number of Data Points	Median	Range <sup>b</sup>	Number of Data Points
Denver-Julesburg, cont.	Tight cont.	Muddy J	D	0.59	.025-0.62	162	--	--	0	230	64-390	3
			V	0.28	0.16-0.62	292	--	--	0	55	9.3-500	129
Fort Worth	Shale	Barnett	H	3.6	1-7.3	23,917	30	21-40	11	920	160-4,200	10,349
			V	1.3	0.4-1.9	3,589	--	--	0	250	170-580	3,318
Green River	Shale	Hilliard-Baxter-Mancos	H	1.7	1.0-5.6	2	--	--	0	37	15-58	7
	Tight	Lance	V	1.3	0.81-3.5	29	3	1-50	31	410	250-580	1,050
			D	1.2	0.76-1.9	180	6	1-17	170	860	360-1,200	1,140
Green River, cont.		Mesaverde	D	0.23	0.16-0.31	73	8	0-37	61	190	150-440	445
			V	0.17	0.081-0.29	14	21	6-83	11	290	140-610	1,081
Illinois	Shale	New Albany	H	--	--	0	--	--	0	--	2,900	2
Michigan	Shale	Antrim	V	--	0.05	1	--	25-75	2	--	4,600	1
Permian	Shale	Avalon & Bone Spring	D	2.2	0.94-4.5	20	13	5-31	16	950	220-2,400	183
			H	1.1	0.73-2.8	17	--	--	0	0	0-2,300	37
		Barnett-Woodford	H	2.1	0.5-4.5	2	--	--	0	--	--	0

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Basin	Resource Type	Unconventional Formation	Drill Type	Fracturing Fluid (Mgal)			Flowback (% of Fracturing Fluid Returned)			Long-Term Produced Water Rates (gpd)		
				Median	Range	Number of Data Points	Median	Range <sup>a</sup>	Number of Data Points	Median	Range <sup>b</sup>	Number of Data Points
Permian, cont.	Shale, cont.	Devonian (TX)	H	0.32	0.13-0.89	10	--	--	0	880	310-1,800	381
			V	0.27	0.12-1.0	16	--	--	0	400	150-3,000	162
		Wolfcamp	H	1.4	1.1-3.9	55	--	--	0	3,000	210-19,000	104
			D	1.3	0.26-1.7	12	16	15-20	3	310	22-8,700	259
			V	0.81	0.078-1.7	60	--	--	0	910	130-1,700	926
	Tight	Spraberry	V	--	1.0	1	--	--	0	870	100-4,000	66
San Juan	Tight	Mesaverde (San Juan)	D	--	--	0	--	--	0	18	12-260	48
		Dakota	V	0.2	0.063-0.22	19	--	--	0	65	29-120	6
			D	0.12	0.07-0.3	52	4	1-40	30	160	41-370	379
TX-LA-MS	Shale	Bossier	H	2.7	1.7-3.6	2	--	--	0	750	610-1,200	25
			V	0.4	0.19-1.7	16	--	--	0	470	180-1,100	1,203
			D	0.28	0.13-0.8	21	--	--	0	320	130-1,300	253
		Haynesville	H	5.3	0.95-15	3,222	5	5-30	3	1,700	84-1,800	1,249
			V	0.61	.14-3.5	9	--	--	0	210	56-850	263
		Tight	Cotton Valley	H	4.2	.25-6.0	30	--	<60	2	770	130-2,700
	D			.48	.084-4.0	24	--	<60	2	950	630-1,800	1801
	V			.28	.019-.94	76	--	<60	2	640	370-1,800	10,717

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Basin	Resource Type	Unconventional Formation	Drill Type	Fracturing Fluid (Mgal)			Flowback (% of Fracturing Fluid Returned)			Long-Term Produced Water Rates (gpd)		
				Median	Range	Number of Data Points	Median	Range <sup>a</sup>	Number of Data Points	Median	Range <sup>b</sup>	Number of Data Points
TX-LA-MS, cont.	Tight, cont.	Travis Peak	H	3.0	0.25-6	2	--	--	0	200	39-1,700	5
			V	0.9	0.2-4	2	--	--	0	980	330-1,800	1,380
Western Gulf	Shale	Eagle Ford	H	5.0	1.0-14	2,485	4	2-8	1,800	110	9.1-250	498
			V	2.9	2.0-4.1	9	--	--	0	--	--	0
		Pearsall	H	3.7	3.3-4.1	2	--	--	0	200	54-370	12
	Tight	Austin Chalk	H	0.94	0.58-1.3	15	--	--	0	720	290-2,400	1,097
		Vicksburg	V	.016	0.084-0.6	20	--	--	0	1,000	650-1,900	937
			D	0.11	0.1-0.13	4	--	--	0	--	--	0
		Wilcox Lobo	H	2.1	0.66-2.6	4	--	--	0	330	62-740	77
			V	0.21	0.06-0.6	14	--	--	0	620	330-1,400	1,514
			D	.058	.056-.076	3	--	--	0	--	--	0
		Olmos	V	--	0.15	2	--	--	0	--	--	0
Williston		Bakken	H	2.0	0.35-10	2,203	19	5-47	206	680	380-1,500	1,739
			V	1.1	.35-2.9	12	--	--	0	1,000	340-3,100	222

"--" indicates no data; H, horizontal well; D, directional well; V, vertical well.

<sup>a</sup> For some formations, if only one data point was reported, the EPA reported it in the range column and did not report a median value.

<sup>b</sup> For some formations, the number of data points was not reported in the data source. In these instances, the EPA reported the number of data points as equal to one, even if the source reported a range and median value.

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## E.2. Produced Water Content

### E.2.1. Introduction

1 In the main text of Chapter 7, we describe aspects of flowback and produced water composition,  
2 including temporal changes in water quality parameters of flowback (Section 7.5) and major classes  
3 of compounds in produced water (Section 7.6). In section 7.7 we describe variability as occurring  
4 on three levels: between different rock types (e.g., coal vs. sandstone), between formations  
5 composed of the same rock types (e.g., Barnett Shale vs. Bakken Shale), and within formations of  
6 the same rock type (e.g., northeastern vs. southwestern Marcellus Shale). In this appendix we  
7 present data from the literature which illustrates the differences among these three variability  
8 levels.

### E.2.2. General Water Quality Parameters

9 As noted in Chapter 7, the EPA identified data characterizing the content of unconventional  
10 flowback and produced water in a total of 12 shale and tight formations and coalbed methane  
11 (CBM) basins. These formations and basins span 18 states. Note that in this subsection we treat all  
12 fluids as produced water. As a consequence, the variability of reported concentrations is likely  
13 higher than if the data could be standardized to a specific point on the flowback-to-produced water  
14 continuum. Table E-2 and Table E-3 provide supporting data on general water quality parameters  
15 of produced water for 12 formations.

**Table E-2. Reported concentrations of general water quality parameters in produced water for unconventional shale and tight formations, presented as: average (minimum–maximum) or *median* (minimum–maximum).**

Parameter	Units	Shales					Tight formations			
		Bakken <sup>a</sup>	Barnett <sup>b</sup>	Fayetteville <sup>c</sup>	Marcellus		Cotton Valley Group <sup>f</sup>	Devonian Sandstone <sup>g</sup>	Mesaverde <sup>f</sup>	Oswego <sup>f</sup>
States	n/a	MT, ND	TX	AR	PA <sup>d</sup>	PA, WV <sup>e</sup>	LA, TX	PA	CO, NM, UT, WY	OK
Acidity	mg/L	-	NC (ND–ND)	-	NC (<5–473)	<b>162</b> (5–925)	-	-	-	-
Alkalinity	mg/L	-	<b>725</b> (215–1,240)	1,347 (811–1,896)	165 (8–577)	<b>99.8</b> (7.5–577)	-	99 (43–194)	-	582 (207–1,220)
Ammonium	mg/L	-	-	-	-	-	89 (40–131)	-	-	-
Bicarbonate	mg/L	291 (122–610)	-	-	-	-	-	524 (ND–8,440)	2,230 (1,281–13,650)	-
Biochemical oxygen demand (BOD)	mg/L	-	<b>582</b> (101–2,120)	-	-	<b>141</b> (2.8–12,400)	-	-	-	-
Carbonate	mg/L	-	-	-	-	-	-	-	227 (ND–1,680)	-
Chloride	mg/L	119,000 (90,000–133,000)	<b>34,700</b> (9,600–60,800)	9,156 (5,507–12,287)	57,447 (64–196,000)	<b>49,000</b> (64.2–196,000)	101,332 (3,167–221,498.7)	132,567 (58,900–207,000)	4,260 (8–75,000)	44,567 (23,000–75,000)
Chemical oxygen demand	mg/L	-	<b>2,945</b> (927–3,150)	-	15,358 (195–36,600)	<b>4,670</b> (195–36,600)	-	-	-	-

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Parameter	Units	Shales					Tight formations			
		Bakken <sup>a</sup>	Barnett <sup>b</sup>	Fayetteville <sup>c</sup>	Marcellus		Cotton Valley Group <sup>f</sup>	Devonian Sandstone <sup>g</sup>	Mesaverde <sup>f</sup>	Oswego <sup>f</sup>
States	n/a	MT, ND	TX	AR	PA <sup>d</sup>	PA, WV <sup>e</sup>	LA, TX	PA	CO, NM, UT, WY	OK
DO	mg/L	-	-	-	-	-	-	0.8 (0.2–2.5)	-	-
DOC	mg/L	-	<b>11.2</b> (5.5–65.3)	-	-	<b>117</b> (3.3–5,960)	-	-	-	-
Hardness as CaCO <sub>3</sub>	mg/L	-	<b>5,800</b> (3,500–21,000)	-	34,000 (630–95,000)	<b>25,000</b> (156–106,000)	-	-	-	-
Oil and grease	mg/L	-	<b>163.5</b> (88.2–1,430)	-	74 (5–802)	<b>16.85</b> (4.7–802)	-	-	-	-
pH	SU	5.87 (5.47–6.53)	<b>7.05</b> (6.5–7.2)	-	6.6 (5.1–8.4)	<b>6.5</b> (4.9–7.9)	-	6.3 (5.5–6.8)	8 (5.8–11.62)	6.3 (6.1–6.4)
Specific conductivity	µS/cm	213,000 (205,000–220,800)	<b>111,500</b> (34,800–179,000)	-	-	<b>183,000</b> (479–763,000)	-	184,800 (118,000–211,000)	-	-
Specific gravity	--	1.13 (1.0961–1.155)	-	-	-	-	-	-	-	-
TDS	mg/L	196,000 (150,000–219,000)	<b>50,550</b> (16,400–97,800)	13,290 (9,972–15,721)	106,390 (680–345,000)	<b>87,800</b> (680–345,000)	164,683 (5,241–356,666)	235,125 (106,000–354,000)	15,802 (1,032–125,304)	73,082 (56,541–108,813)
Total Kjeldahl nitrogen	mg/L	-	<b>171</b> (26–298)	-	-	<b>94.9</b> (5.6–312)	-	-	-	-

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Parameter	Units	Shales					Tight formations			
		Bakken <sup>a</sup>	Barnett <sup>b</sup>	Fayetteville <sup>c</sup>	Marcellus		Cotton Valley Group <sup>f</sup>	Devonian Sandstone <sup>g</sup>	Mesaverde <sup>f</sup>	Oswego <sup>f</sup>
States	n/a	MT, ND	TX	AR	PA <sup>d</sup>	PA, WV <sup>e</sup>	LA, TX	PA	CO, NM, UT, WY	OK
TOC	mg/L	-	<b>9.75</b> (6.2–36.2)	-	160 (1.2–1,530)	<b>89.2</b> (1.2–5,680)	198 (184–212)	-	-	-
Total suspended solids	mg/L	-	<b>242</b> (120–535)	-	352 (4–7,600)	<b>127</b> (6.8–3,220)	-	-	-	-
Turbidity	NTU	-	<b>239</b> (144–314)	-	-	<b>126</b> (2.3–1,540)	-	-	-	-

n/a, not applicable; -, no value available; NC, not calculated; ND, not detected., SU= standard units, ***bolded italic*** numbers are medians

<sup>a</sup> [Stepan et al. \(2010\)](#). *n* = 3. Concentrations were calculated based on Stepan et al.'s raw data. Samples had charge balance errors of 1.74, -0.752, and -0.220%

<sup>b</sup> [Hayes and Severin \(2012b\)](#). *n* = 16. This data source reported concentrations without direct presentation of raw data.

<sup>c</sup> [Warner et al. \(2013\)](#). *n* = 6. Concentrations were calculated based on Warner et al.'s raw data. Both flowback and produced water included.

<sup>d</sup> [Barbot et al. \(2013\)](#). *n* = 134–159. This data source reported concentrations without direct presentation of raw data.

<sup>e</sup> [Hayes \(2009\)](#). *n* = 31–67. Concentrations were calculated based on Hayes's raw data. Both flowback and produced water included. Non-detects and contaminated blanks omitted.

<sup>f</sup> [Blondes et al. \(2014\)](#). Cotton Valley Group, *n*=2; Mesa Verde, *n* = 1–407; Oswego, *n* = 4–30. Concentrations were calculated based on raw data presented in the U.S. Geological Survey (USGS) National Produced Water Database v2.0.

<sup>g</sup> [Dresel and Rose \(2010\)](#). *n* = 3–15. Concentrations were calculated based on Dresel and Rose's raw data.

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**Table E-3. Reported concentrations of general water quality parameters in produced water for unconventional coalbed basins, presented as: average (minimum–maximum).**

Parameter	Units	Black Warrior <sup>a</sup>	Powder River <sup>b</sup>	Raton <sup>b</sup>	San Juan <sup>b</sup>
States	n/a	AL, MS	MT, WY	CO, NM	AZ, CO, NM, UT
Alkalinity	mg/L	355 (3–1,600)	1,384 (653–2,672)	1,107 (130–2,160)	3,181 (51–11,400)
Ammonium	mg/L	3.60 (0.16–8.91)	-	-	-
Bicarbonate	mg/L	427 (2–1,922)	1,080 (236–3,080)	1,124 (127–2,640)	3,380 (117–13,900)
Carbonate	mg/L	3 (0–64)	2.17 (0.00–139.0)	51.30 (1.30–316.33)	40.17 (0.00–1,178)
Chloride	mg/L	9,078 (11–42,800)	21 (BDL–282)	787 (4.8–8,310)	624 (BDL–20,100)
Chemical oxygen demand	mg/L	830 (0–10,500)	-	-	-
Dissolved oxygen	mg/L	-	1.07 (0.11–3.48)	0.39 (0.01–3.52)	0.51 (0.04–1.69)
DOC	mg/L	3.37 (0.53–61.41)	3.18 (1.09–8.04)	1.26 (0.30–8.54)	3.21 (0.89–11.41)
Hardness as CaCO <sub>3</sub>	mg/L	871 (3–6,150)	-	-	-
Hydrogen sulfide	mg/L	-	-	4.41 (BDL–190.0)	23.00 (23.00–23.00)
Oil and grease	mg/L	-	-	9.10 (0.60–17.6)	-
pH	SU	7.5 (5.3–9.0)	7.71 (6.86–9.16)	8.19 (6.90–9.31)	7.82 (5.40–9.26)
Phosphate	mg/L	0.435 (0.026–3.570)	BDL (BDL–BDL)	0.04 (BDL–1.00)	1.89 (BDL–9.42)
Specific conductivity	μS/cm	20,631 (718–97,700)	1,598 (413–4,420)	3,199 (742–11,550)	5,308 (232–18,066)
TDS	mg/L	14,319 (589–61,733)	997 (252–2,768)	2,512 (244–14,800)	4,693 (150–39,260)
Total Kjeldahl nitrogen	mg/L	6.08 (0.15–38.40)	0.48 (BDL–4.70)	2.61 (BDL–26.10)	0.46 (BDL–3.76)
TOC	mg/L	6.03 (0.00–103.00)	3.52 (2.07–6.57)	1.74 (0.25–13.00)	2.91 (0.95–9.36)
Total suspended solids	mg/L	78 (0–2,290)	11.0 (1.4–72.7)	32.3 (1.0–580.0)	47.2 (1.4–236.0)
Turbidity	NTU	74 (0–539)	8.2 (0.7–57.0)	4.5 (0.3–25.0)	61.6 (0.8–810.0)

n/a, not applicable; -, no value available; BDL, below detection limit.

<sup>a</sup> [DOE \(2014\)](#).  $n = 206$ . Concentrations were calculated based on raw data presented in the reference.

<sup>b</sup> [Dahm et al. \(2011\)](#). Powder River,  $n = 31$ ; Raton,  $n = 40$ ; San Juan,  $n = 20$ . This data source reported concentrations without presentation of raw data.

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### E.2.3. Salinity and Inorganics

1 Table E-4 and Table E-5 provide supporting data on salinity and inorganic constituents of produced  
2 water for 12 formations.

#### E.2.3.1. Processes Controlling Salinity and Inorganics Concentrations

3 Multiple mechanisms likely control elevated salt concentrations in flowback and produced water  
4 and are largely dependent upon post-injection fluid interactions and the formation's stratigraphic  
5 and hydrogeologic environment ([Barbot et al., 2013](#)). High inorganic ionic loads observed in  
6 flowback and produced water are expressed as TDS.

7 Subsurface brines or formation waters are saline fluids associated with the targeted formation.  
8 Shale and sandstone brines are typically much more saline than coalbed waters. After hydraulic  
9 fracturing fluids are injected into the subsurface, the injected fluids (which are typically not sources  
10 of high TDS) mix with in situ brines, which typically contain high ionic loads ([Haluszczak et al.,  
11 2013](#)).

12 Deep brines, present in over- or underlying strata, may naturally migrate into targeted formations  
13 over geologic time or artificially intrude if a saline aquifer is breached during hydraulic fracturing  
14 ([Chapman et al., 2012](#); [Maxwell, 2011](#); [Blauch et al., 2009](#)). Whether it is through natural or induced  
15 intrusion, saline fluids may contact the producing formation and introduce novel salinity sources to  
16 the produced water ([Chapman et al., 2012](#)).

17 The dissolution salts associated with formation solids both increases TDS concentrations and alters  
18 formation porosity and permeability ([Blauch et al., 2009](#)). Additionally, the mobilization of connate  
19 fluids (deposition-associated pore fluids) and formation fluids during hydraulic fracturing likely  
20 contributes to increased TDS levels ([Dresel and Rose, 2010](#); [Blauch et al., 2009](#)). Despite the general  
21 use of fresh water for hydraulic fracturing fluid, some elevated salts in produced water may result  
22 from the use of reused saline flowback or produced water as a hydraulic fracturing base fluid  
23 ([Hayes, 2009](#)).

**Table E-4. Reported concentrations (mg/L) of inorganic constituents contributing to salinity in unconventional shale and tight formations produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum).**

Parameter	Shale					Tight Formations			
	Bakken <sup>a</sup>	Barnett <sup>b</sup>	Fayetteville <sup>c</sup>	Marcellus		Cotton Valley Group <sup>f</sup>	Devonian Sandstone <sup>g</sup>	Mesaverde <sup>f</sup>	Oswego <sup>f</sup>
States	MT, ND	TX	AR	PA <sup>d</sup>	PA, WV <sup>e</sup>	LA, TX	PA	CO, NM, UT, WY	OK
<b>Bromide</b>	-	<b>589</b> (117–798)	111 (96–144)	511 (0.2–1,990)	<b>512</b> (15.8–1,990)	498 (32–1,338)	1,048 (349–1,350)	-	-
<b>Calcium</b>	9,680 (7,540–13,500)	<b>1,600</b> (1,110–6,730)	317 (221–386)	7,220 (38–41,000)	<b>7,465</b> (173–33,000)	19,998 (181–51,400)	20,262 (8,930–34,400)	212 (1.01–4,580)	5,903 (3,609–8,662)
<b>Chloride</b>	119,000 (90,000–133,000)	<b>34,700</b> (9,600–60,800)	9,156 (5,507–12,287)	57,447 (64–196,000)	<b>49,000</b> (64.2–196,000)	101,332 (3,167–221,498.7)	132,567 (58,900–207,000)	4,260 (8–75,000)	44,567 (23,000–75,000)
<b>Fluoride</b>	-	<b>3.8</b> (3.5–12.8)	-	-	<b>0.975</b> (0.077–32.9)	-	-	-	-
<b>Iodine</b>	-	-	-	-	-	20 (1–36)	39 (11–56)	1.01 (1.01–1.01)	-
<b>Nitrate as N</b>	-	-	NC (ND–ND)	-	<b>1.7</b> (0.65–15.9)	-	-	0.6 (0.6–0.6)	-
<b>Nitrite as N</b>	-	<b>4.7</b> (3.5–38.1)	-	-	<b>11.8</b> (1.1–146)	-	-	-	-
<b>Phosphorus</b>	NC (ND–0.03)	<b>0.395</b> (0.19–0.7)	-	-	<b>0.3</b> (0.08–21.8)	-	-	-	-
<b>Potassium</b>	2,970 (0–5,770)	<b>316</b> (80–750)	-	-	<b>337</b> (38–3,950)	1,975 (8–7,099)	858 (126–3,890)	160 (4–2,621)	-

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Parameter	Shale					Tight Formations			
	Bakken <sup>a</sup>	Barnett <sup>b</sup>	Fayetteville <sup>c</sup>	Marcellus		Cotton Valley Group <sup>f</sup>	Devonian Sandstone <sup>g</sup>	Mesaverde <sup>f</sup>	Oswego <sup>f</sup>
States	MT, ND	TX	AR	PA <sup>d</sup>	PA,WV <sup>e</sup>	LA, TX	PA	CO, NM, UT, WY	OK
Silica	7 (6.41–7)	-	52 (13–160)	-	-	4 (4–4)	-	-	-
Sodium	61,500 (47,100–74,600)	<b>18,850</b> (4,370–28,200)	3,758 (3,152–4,607)	21,123 (69–117,000)	<b>21,650</b> (63.8–95,500)	39,836 (1,320–85,623.24)	58,160 (24,400–83,300)	5,828 (132–48,817)	19,460 (13,484–31,328)
Sulfate	660 (300–1,000)	<b>709</b> (120–1,260)	NC (ND–3)	71 (0–763)	<b>58.9</b> (2.4–348)	407 (ND–2,200.46)	20 (1–140)	837 (ND–14,612)	183 (120–271)
Sulfide	-	NC (ND–ND)	-	-	<b>3.2</b> (1.6–5.6)	-	0.7 (0.1–2.5)	-	-
Sulfite	-	-	-	-	<b>12.4</b> (5.2–73.6)	-	-	-	-
TDS	196,000 (150,000–219,000)	<b>50,550</b> (16,400–97,800)	13,290 (9,972–15,721)	106,390 (680–345,000)	<b>87,800</b> (680–345,000)	164,683 (5,241–356,666)	235,125 (106,000–354,000)	15,802 (1,032–125,304)	73,082 (56,541–108,813)

-, no value available; NC, not calculated; ND, not detected. **Bolded italic** numbers are medians.

<sup>a</sup> [Stepan et al. \(2010\)](#).  $n = 3$ . Concentrations were calculated based on Stepan et al.'s raw data. Samples had charge balance errors of 1.74, -0.752, and -0.220%

<sup>b</sup> [Hayes and Severin \(2012b\)](#).  $n = 16$ . This data source reported concentrations without presentation of raw data.

<sup>c</sup> [Warner et al. \(2013\)](#).  $n = 6$ . Concentrations were calculated based on Warner et al.'s raw data. Both flowback and produced water included.

<sup>d</sup> [Barbot et al. \(2013\)](#).  $n = 134–159$ . This data source reported concentrations without presentation of raw data.

<sup>e</sup> [Hayes \(2009\)](#).  $n = 8–65$ . Concentrations were calculated based on Hayes's raw data. Both flowback and produced water included. Non-detects and contaminated blanks omitted.

<sup>f</sup> [Blondes et al. \(2014\)](#) Cotton Valley Group,  $n = 2$ ; Mesa Verde,  $n = 1–407$ ; Oswego,  $n = 4–30$ . Concentrations were calculated based on raw data presented in the USGS National Produced Water Database v2.0.

<sup>g</sup> [Dresel and Rose \(2010\)](#).  $n = 3–15$ . Concentrations were calculated based on Dresel and Rose's raw data.

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**Table E-5. Reported concentrations (mg/L) of inorganic constituents contributing to salinity in produced water for unconventional CBM basins, presented as: average (minimum–maximum).**

Parameter	Black Warrior <sup>a</sup>	Powder River <sup>b</sup>	Raton <sup>b</sup>	San Juan <sup>b</sup>
State	AL, MS	MT, WY	CO, NM	AZ, CO, NM, UT
Barium	45.540 (0.136–352)	0.61 (0.14–2.47)	1.67 (BDL–27.40)	10.80 (BDL–74.0)
Boron	0.185 (0–0.541)	0.17 (BDL–0.39)	0.36 (BDL–4.70)	1.30 (0.21–3.45)
Bromide	-	0.09 (BDL–0.26)	4.86 (0.04–69.60)	9.77 (BDL–43.48)
Calcium	218 (0–1,640)	32.09 (2.00–154.0)	14.47 (0.81–269.0)	53.29 (1.00–5,530)
Chloride	9,078 (11–42,800)	21 (BDL–282)	787 (4.8–8,310)	624 (BDL–20,100)
Fluoride	6.13 (0.00–22.60)	1.57 (0.40–4.00)	4.27 (0.59–20.00)	1.76 (0.58–10.00)
Magnesium	68.12 (0.18–414.00)	14.66 (BDL–95.00)	3.31 (0.10–56.10)	15.45 (BDL–511.0)
Nitrate	8.70 (0.00–127.50)	-	-	-
Nitrite	0.03 (0.00–2.08)	-	-	-
Phosphorus	0.32 (0.00–5.76)	-	-	-
Potassium	12.02 (0.46–74.00)	11.95 (BDL–44.00)	6.37 (BDL–29.40)	26.99 (BDL–970.0)
Silica	8.66 (1.04–18.10)	6.46 (4.40–12.79)	7.05 (4.86–10.56)	12.37 (3.62–37.75)
Sodium	4,353 (126–16,700)	356 (12–1,170)	989 (95–5,260)	1,610 (36–7,834)
Strontium	11.354 (0.015–142.000)	0.60 (0.10–1.83)	5.87 (BDL–47.90)	5.36 (BDL–27.00)
Sulfate	5.83 (0.00–302.00)	5.64 (BDL–300.0)	14.75 (BDL–253.00)	25.73 (BDL–1,800)
TDS	14,319 (589–61,733)	997 (252–2,768)	2,512 (244–14,800)	4,693 (150–39,260)

-, no value available; BDL, below detection limit.

<sup>a</sup> [DOE \(2014\)](#).  $n = 206$ . Concentrations were calculated based on the authors' raw data.

<sup>b</sup> [Dahm et al. \(2011\)](#). Powder River,  $n = 31$ ; Raton,  $n = 40$ ; San Juan,  $n = 20$ . This data source reported concentrations without presentation of raw data.

#### E.2.4. Metals and Metalloids

- 1 Table E-6 and Table E-7 provide supporting data on metal constituents of produced water for 12
- 2 formations.

**Table E-6. Reported concentrations (mg/L) of metals and metalloids from unconventional shale and tight formation produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum).**

Note that calcium, potassium, and sodium appear in Table E-4.

Parameter	Shale					Tight Formation			
	Bakken <sup>a</sup>	Barnett <sup>b</sup>	Fayetteville <sup>c</sup>	Marcellus		Cotton Valley Group <sup>f</sup>	Devonian Sandstone <sup>g</sup>	Mesaverde <sup>f</sup>	Oswego <sup>f</sup>
States	MT, ND	TX	AR	PA <sup>d</sup>	PA, WV <sup>e</sup>	LA, TX	PA	CO, NM, UT, WY	OK
Aluminum	-	<b>0.43</b> (0.37–2.21)	-	-	<b>2.57</b> (0.22–47.2)	-	-	-	-
Antimony	-	NC (ND–ND)	-	-	<b>0.028</b> (0.018–0.038)	-	-	-	-
Arsenic	-	NC (ND–ND)	-	-	<b>0.101</b> (0.013–0.124)	-	-	-	-
Barium	10 (0–24.6)	<b>3.6</b> (0.93–17.9)	4 (3–5)	2,224 (0.24–13,800)	<b>542.5</b> (2.590–13,900)	160 (ND–400.52)	1,488 (7–4,370)	139 (4–257)	-
Beryllium	-	NC (ND–ND)	-	-	-	-	-	-	-
Boron	116 (39.9–192)	<b>30.3</b> (7.0–31.9)	4.800 (2.395–21.102)	-	<b>12.2</b> (0.808–145)	37 (2–100)	-	10 (1–14.2)	-
Cadmium	-	NC (ND–ND)	-	-	-	-	-	-	-
Chromium	-	<b>0.03</b> (0.01–0.12)	-	-	<b>0.079</b> (0.011–0.567)	-	-	-	-
Cobalt	-	<b>0.01</b> (0.01–0.01)	-	-	-	-	-	-	-

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Parameter	Shale					Tight Formation			
	Bakken <sup>a</sup>	Barnett <sup>b</sup>	Fayetteville <sup>c</sup>	Marcellus		Cotton Valley Group <sup>f</sup>	Devonian Sandstone <sup>g</sup>	Mesaverde <sup>f</sup>	Oswego <sup>f</sup>
States	MT, ND	TX	AR	PA <sup>d</sup>	PA, WV <sup>e</sup>	LA, TX	PA	CO, NM, UT, WY	OK
Copper	NC (ND-0.21)	<b>0.29</b> (0.06-0.52)	-	-	<b>0.506</b> (0.253-4.150)	0.7 (0.48-1)	0.04 (0.01-0.13)	-	-
Iron	96 (ND-120)	<b>24.9</b> (12.1-93.8)	7 (1-13)	-	<b>53.65</b> (2.68-574)	-	188 (90-458)	9 (1-29)	61 (41-78)
Lead	-	<b>0.02</b> (0.01-0.02)	-	-	<b>0.066</b> (0.003-0.970)	-	0.02 (0.01-0.04)	-	-
Lithium	-	<b>19.0</b> (2.56-37.4)	9.825 (2.777-28.145)	-	<b>53.85</b> (3.410-323)	23 (1-53)	97.8 (20.2-315)	3 (1-33)	-
Magnesium	1,270 (630-1,750)	<b>255</b> (149-755)	61 (47-75)	632 (17-2,550)	<b>678</b> (40.8-2,020)	1,363 (27-3,712.98)	2,334 (797-3,140)	74 (1-2,394)	753 (486-1,264)
Manganese	7 (4-10.2)	<b>0.86</b> (0.25-2.20)	2 (2-3)	-	<b>2.825</b> (0.369-18.600)	30.33 (30.33-30.33)	19 (5.6-68)	-	-
Mercury	-	NC (ND-ND)	-	-	<i>0.00024</i>	-	-	-	-
Molybdenum	NC (ND-<0.2)	<b>0.02</b> (0.02-0.03)	-	-	-	-	-	-	-
Nickel	-	<b>0.04</b> (0.03-0.05)	-	<b>0.1815</b> (0.007-0.137)	<b>0.419</b> (0.068-0.769)	-	-	-	-
Selenium	-	<b>0.03</b> (0.03-0.04)	-	-	<i>0.004</i>	-	-	-	-
Silver	-	-	-	-	<b>4</b> (3-6)	-	-	-	-

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Parameter	Shale					Tight Formation			
	Bakken <sup>a</sup>	Barnett <sup>b</sup>	Fayetteville <sup>c</sup>	Marcellus		Cotton Valley Group <sup>f</sup>	Devonian Sandstone <sup>g</sup>	Mesaverde <sup>f</sup>	Oswego <sup>f</sup>
States	MT, ND	TX	AR	PA <sup>d</sup>	PA, WV <sup>e</sup>	LA, TX	PA	CO, NM, UT, WY	OK
Strontium	764 (518–1,010)	<b>529</b> (48–1,550)	27 (14–49)	1,695 (0.6–8,460)	<b>1,240</b> (0.580–8,020)	2,312 (39–9,770)	3,890 (404–13,100)	-	-
Thallium	-	NC (ND–0.14)	-	-	<i>0.168</i>	-	-	-	-
Tin	-	NC (ND–ND)	-	-	-	-	-	-	-
Titanium	-	<b>0.02</b> (0.02–0.03)	-	-	-	-	-	-	-
Zinc	7 (2–11.3)	<b>0.15</b> (0.10–0.36)	-	-	<b>0.391</b> (0.087–247)	-	0.20 (0.03–1.26)	-	-

-, no value available; NC, not calculated; ND, not detected; BDL, below detection limit. ***Bolded italic*** numbers are medians.

<sup>a</sup> [Stepan et al. \(2010\)](#). *n* = 3. Concentrations were calculated based on Stepan et al.'s raw data.

<sup>b</sup> [Hayes and Severin \(2012b\)](#). *n* = 16. This data source reported concentrations without presentation of raw data.

<sup>c</sup> [Warner et al. \(2013\)](#). *n* = 6. Concentrations were calculated based on Warner et al.'s raw data. Both flowback and produced water included.

<sup>d</sup> [Barbot et al. \(2013\)](#). *n* = 134–159. This data source reported concentrations without presentation of data.

<sup>e</sup> [Hayes \(2009\)](#). *n* = 48. Concentrations were calculated based on Hayes's raw data. Both flowback and produced water included. Non-detects and contaminated blanks omitted.

<sup>f</sup> [Blondes et al. \(2014\)](#). Cotton Valley Group, *n* = 2; Mesa Verde, *n* = 1–407; Oswego, *n* = 4–30. Concentrations were calculated based on raw data presented in the USGS National Produced Water Database v2.0.

<sup>g</sup> [Dresel and Rose \(2010\)](#). *n* = 3–15. Concentrations were calculated based on Dresel and Rose's raw data.

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**Table E-7. Reported concentrations (mg/L) of metals and metalloids from unconventional coalbed produced water, presented as: average (minimum–maximum).**

Parameter	Black Warrior <sup>a</sup>	Powder River <sup>b</sup>	Raton <sup>b</sup>	San Juan <sup>b</sup>
States	AL, MS	MT, WY	CO, NM	AZ, CO, NM, UT
Aluminum	0.037 (0–0.099)	0.018 (BDL–0.124)	0.193 (BDL–2,900)	0.069 (BDL–0.546)
Antimony	0.006 (0.00–0.022)	BDL (BDL–BDL)	BDL (BDL–BDL)	BDL (BDL–BDL)
Arsenic	0.002 (0.0–0.085)	0.001 (BDL–0.004)	0.010 (BDL–0.060)	0.001 (BDL–0.020)
Barium	45.540 (0.136–352)	0.61 (0.14–2.47)	1.67 (BDL–27.40)	10.80 (BDL–74.0)
Beryllium	0.0 (0.0–0.008)	BDL (BDL–BDL)	BDL (BDL–BDL)	BDL (BDL–BDL)
Boron	0.185 (0–0.541)	0.17 (BDL–0.39)	0.36 (BDL–4.70)	1.30 (0.21–3.45)
Cadmium	0.001 (0.00–0.015)	BDL (BDL–0.002)	0.002 (BDL–0.003)	0.002 (BDL–.006)
Calcium	218 (0–1,640)	32.09 (2.00–154.0)	14.47 (0.81–269.0)	53.29 (1.00–5,530)
Cesium	0.011 (0.0–0.072)	-	-	-
Chromium	0.002 (0.0–0.351)	0.012 (BDL–0.250)	0.105 (BDL–3.710)	0.002 (BDL–0.023)
Cobalt	0.023 (0.00–0.162)	BDL (BDL–BDL)	0.001 (BDL–0.018)	0.001 (BDL–0.017)
Copper	0.001 (0.0–0.098)	0.078 (BDL–1.505)	0.091 (BDL–4.600)	0.058 (BDL–0.706)
Iron	8.956 (0.045–93.100)	1.55 (BDL–190.0)	7.18 (0.09–95.90)	6.20 (BDL–258.0)
Lead	0.008 (0.00–0.250)	BDL (BDL–BDL)	0.023 (BDL–0.233)	0.023 (BDL–0.390)
Lithium	1.157 (0–8.940)	0.13 (BDL–0.34)	0.32 (0.01–1.00)	1.61 (0.21–4.73)
Magnesium	68.12 (0.18–414.00)	14.66 (BDL–95.00)	3.31 (0.10–56.10)	15.45 (BDL–511.0)
Manganese	0.245 (0.006–4.840)	0.02 (BDL–0.16)	0.11 (0.01–2.00)	0.19 (BDL–1.34)
Mercury	0.000 (0.000–0.000)	-	-	-
Molybdenum	0.002 (0–0.083)	0.005 (BDL–0.029)	0.002 (BDL–0.035)	0.020 (BDL–0.040)
Nickel	0.015 (0.0–0.358)	0.141 (BDL–2.61)	0.015 (0.004–0.11)	0.020 (BDL–0.13)
Potassium	12.02 (0.46–74.00)	11.95 (BDL–44.00)	6.37 (BDL–29.40)	26.99 (BDL–970.0)
Rubidium	0.013 (0.0–0.114)	-	-	-
Selenium	0.002 (0.00–0.063)	0.006 (BDL–0.046)	0.017 (BDL–0.100)	0.018 (BDL–0.067)
Silver	0.015 (0.0–0.565)	0.003 (0.003–0.003)	0.015 (BDL–0.140)	BDL (BDL–BDL)
Sodium	4,353 (126–16,700)	356 (12–1,170)	989 (95–5,260)	1,610 (36–7,834)
Strontium	11.354 (0.015–142.000)	0.60 (0.10–1.83)	5.87 (BDL–47.90)	5.36 (BDL–27.00)
Thallium	-	-	-	-
Tin	0.00 (0.00–0.009)	0.006 (BDL–0.028)	0.008 (BDL–0.021)	0.017 (BDL–0.039)
Titanium	0.003 (0.0–0.045)	BDL (BDL–0.002)	BDL (BDL–0.002)	0.004 (BDL–0.020)

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Parameter	Black Warrior <sup>a</sup>	Powder River <sup>b</sup>	Raton <sup>b</sup>	San Juan <sup>b</sup>
States	AL, MS	MT, WY	CO, NM	AZ, CO, NM, UT
Vanadium	0.001 (0.0–0.039)	BDL (BDL–BDL)	0.001 (BDL–0.013)	BDL (BDL–BDL)
Zinc	0.024 (0.0–0.278)	0.063 (BDL–0.390)	0.083 (0.010–3.900)	0.047 (0.005–0.263)

-, no value available; BDL, below detection limit.

<sup>a</sup> DOE (2014).  $n = 206$ . Concentrations were calculated based on the authors' raw data.

<sup>b</sup> Dahm et al. (2011). Powder River,  $n = 31$ ; Raton,  $n = 40$ ; San Juan,  $n = 20$ . This data source reported concentrations without presentation of raw data.

#### E.2.4.1. Processes Controlling Mineral Precipitation and Dissolution

1 Hydraulic fracturing treatments introduce fluids into the subsurface that are not in equilibrium  
 2 with respect to formation mineralogy. Subsurface geochemical equilibrium modeling and  
 3 saturation indices are therefore used to assess the solution chemistry of unconventional produced  
 4 water and the subsequent likelihood of precipitation and dissolution reactions (Engle and Rowan,  
 5 2014; Barbot et al., 2013). Dissolution and precipitation reactions between fracturing fluids,  
 6 formation solids, and formation water contribute to the chemistry of flowback and produced water.

7 For example, early flowback fluids may be under-saturated with respect to certain constituents or  
 8 minerals associated with formation solids. Through time, as fluid-rock geochemistry returns to  
 9 equilibrium, formation minerals will dissolve into solution and return in flowback.

10 Depending upon the formation chemistry and composition of the hydraulic fracturing fluid, the  
 11 hydraulic fracturing fluid may initially have a lower ionic strength than existing formation fluids.  
 12 Consequently, salts, carbonate, sulfate, and silicate minerals may undergo dissolution or  
 13 precipitation. Proppants may also undergo dissolution or serve as nucleation sites for precipitation  
 14 (McLin et al., 2011).

15 Currently, relatively little literature quantitatively explores subsurface dissolution and  
 16 precipitation reactions between hydraulic fracturing fluids and formation solids and water.  
 17 However, the processes that take place will likely be a function of the solubilities of the minerals,  
 18 the chemistry of the fluid, pH, redox conditions, and temperature.

19 Documented dissolution processes in unconventional resources include the dissolution of feldspar  
 20 followed by sodium enrichment in coalbed produced water (Rice et al., 2008). Dissolution of  
 21 barium-rich minerals (barite ( $\text{BaSO}_4$ ) and witherite ( $\text{BaCO}_3$ )), and strontium-rich minerals (celestite  
 22 ( $\text{SrSO}_4$ ) and strontianite ( $\text{SrCO}_3$ )) are known to enrich shale produced waters in barium and  
 23 strontium (Chapman et al., 2012).

24 Known precipitation processes in unconventional resources include the precipitation of carbonate  
 25 and subsequent reduction of calcium and magnesium concentrations in coalbed produced water  
 26 (Rice et al., 2008). Additionally, calcium carbonate precipitation is suspected to cause declines in pH  
 27 and alkalinity levels in shale produced water (Barbot et al., 2013).

1 The subsurface processes associated with fluid-rock interactions take place over a scale of weeks to  
2 months through the generation of flowback and produced water. Note that the types and extent of  
3 subsurface dissolution and precipitation reactions change with time, from injection through  
4 flowback and production. For instance, [Engle and Rowan \(2014\)](#) found that early Marcellus Shale  
5 flowback was under-saturated with respect to gypsum ( $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ ), halite ( $\text{NaCl}$ ), celestite,  
6 strontianite, and witherite, indicating that these minerals would dissolve in the subsurface. Fluids  
7 were oversaturated with respect to barite. Saturation indices for gypsum, halite, celestite, and  
8 barite all increased during production. Knowing when dissolution and precipitation will likely  
9 occur is important, because dissolution and precipitation of minerals change formation  
10 permeability and porosity, which can affect production ([André et al., 2006](#)).

11 Additionally, pyrite ( $\text{FeS}_2$ ) is an important minor mineral in reduced sedimentary rocks. Pyrite is  
12 the primary form of sulfur and iron occurrence in shales ([Leventhal and Hosterman, 1982](#)) and is  
13 also a common mineral phase generated in coals in which organic matter is closely associated  
14 ([Ward, 2002](#)). Pyrite content in shales can vary from less than 1% to several percent ([Chermak and](#)  
15 [Schreiber, 2014](#); [Vulgamore et al., 2007](#)). Researchers have found a strong association of trace  
16 metals (i.e., nickel, copper, cadmium, chromium, cobalt, lead, selenium, vanadium, and zinc) with  
17 pyrite in shales ([Chermak and Schreiber, 2014](#); [Tuttle et al., 2009](#); [Leventhal and Hosterman, 1982](#)).

18 Although studies considering pyrite oxidation within the context of hydraulic fracturing are  
19 currently lacking, it is likely that the introduction of oxygenated fluids to freshly exposed surfaces  
20 in the subsurface during hydraulic fracturing can initiate limited, short-term pyrite oxidation or  
21 dissolution. Pyrite dissolution may increase iron and trace element concentrations and acidity in  
22 produced waters ([Nordstrom and Alpers, 1999](#); [Moses and Herman, 1991](#)).

23 The extent to which the oxidative dissolution of pyrite would exert a control on post-injection  
24 subsurface fluid chemistry is unknown, although an ongoing U.S. Geological Survey (USGS) study  
25 anticipates it may be more significant than previously hypothesized ([Li and Brantley, 2011](#)).  
26 Regardless, relative to other reactions contributing to the composition of flowback and produced  
27 water (i.e., dissolution of salts), pyrite oxidation appears to be less significant. Ultimately, reactions  
28 resulting from temporary changes in subsurface redox conditions will be less important relative to  
29 other reactions that are less redox-dependent.

## **E.2.5. Naturally Occurring Radioactive Material (NORM) and Technically Enhanced Naturally Occurring Radioactive Material (TENORM)**

### ***E.2.5.1. Formation Solids Levels of NORM***

30 Elevated uranium levels in formation solids have been used to identify potential areas of natural  
31 gas production for decades ([Fertl and Chilingar, 1988](#)). Marine black shales are estimated to contain  
32 an average of 5–20 ppm uranium depending on depositional conditions, compared to an average of  
33 less than 5 ppm among all shales ([USGS, 1961](#)). Shales that bear significant levels of uranium  
34 include the Barnett in Texas, the Woodford in Oklahoma, the New Albany in the Illinois Basin, the  
35 Chattanooga Shale in the southeastern United States, and a group of black shales in Kansas and  
36 Oklahoma ([Swanson, 1955](#)).

1 [Bank et al. \(2012\)](#) identified Marcellus samples with uranium ranging from 4–72 ppm, with an  
2 average of 30 ppm. Additionally, shale samples taken from three counties within the Marcellus  
3 Shale had uranium concentrations ranging from 8 to 84 ppm ([BTGS, 2011](#); [Hatch and Leventhal,  
4 1981](#)). [Chermak and Schreiber \(2014\)](#) compiled mineralogy and trace element data available in the  
5 literature for nine U.S. hydrocarbon-producing shales. In this combined data set, uranium levels  
6 among different shale plays were found to vary over three orders of magnitude, with samples of the  
7 Utica Shale containing approximately 0–5 ppm uranium and samples of the Woodford Shale  
8 containing uranium in the several-hundred-ppm range.

9 [Vine \(1956\)](#) reported that the principal uranium-bearing coal deposits of the United States are  
10 found in Cretaceous and Tertiary formations in the northern Great Plains and Rocky Mountains; in  
11 some areas of the West, coal deposits have been found with uranium concentrations in the range of  
12 thousands of ppm or greater. In contrast, most Mississippian, Pennsylvanian, and Permian coals in  
13 the north-central and eastern United States contain less than 10 ppm uranium, rarely containing  
14 50 ppm or more.

#### **E.2.5.2. Produced Water Levels of TENORM**

15 Background data on NORM in the Marcellus Shale and Devonian sandstones are given in Table E-8.

**Table E-8. Reported concentrations (in pCi/L) of radioactive constituents in unconventional shale and sandstone produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum).**

Parameter	Marcellus			Devonian Sandstone <sup>a</sup>		
	States	NY, PA <sup>b</sup>	PA NORM STUDY ( <a href="#">PA DEP, 2015</a> )			
			Flowback <sup>c</sup>		Conventional Produced Water <sup>d</sup>	Unconventional Produced Water <sup>e</sup>
Gross alpha		<b>6,845</b> (ND–123,000)	<b>10,700</b> (288–71,000)	<b>1,835</b> (465–2,570)	<b>11,300</b> (2,240–41,700)	-
Gross beta		<b>1,170</b> (ND–12,000)	<b>2,400</b> (742–21,300)	<b>909</b> (402–1,140)	<b>3,445</b> (1.5–7,600)	-
Radium-226		<b>1,869</b> (ND–16,920)	<b>4,500</b> (551–25,500)	<b>243</b> (81 – 819)	<b>6,300</b> (1,700–26,600)	<b>2,367</b> (200–5,000)
Radium-228		<b>557</b> (ND–2,589)	<b>633</b> (248–1,740)	<b>128</b> (26 – 896)	<b>941</b> (366–1,900)	-
Total Radium		<b>2,530</b> (0.192–18,045)	-	<b>371</b> (107 – 1,715)	<b>7,180</b> (2,336–28,500)	-
Uranium <sup>235</sup>		1 (ND–20)	-	-	-	-
Uranium <sup>238</sup>		42 (ND–497)	-	-	-	-

n/a, not applicable; -, no value available; BDL, below detection limit. ***Bolded italic*** numbers are medians.

<sup>a</sup> [Dresel and Rose \(2010\)](#). *n* = 3. Concentrations presented were calculated based on Dresel and Rose's raw data.

<sup>b</sup> [Rowan et al. \(2011\)](#). *n* = 51. Concentrations presented were calculated based on Rowan et al.'s raw data for Marcellus samples. Uranium data from Barbot et al. (2013) *n* = 14.

<sup>c</sup> [PA DEP \(2015\)](#). *n* = 9. Data reported in Table 3-14.

<sup>d</sup> [PA DEP \(2015\)](#). *n* = 9. Values calculated from Table 3-15 for unfiltered samples.

<sup>e</sup> [PA DEP \(2015\)](#). *n* = 4. Values calculated from Table 3-15 for unfiltered samples.

### **E.2.5.3. Mobilization of Naturally Occurring Radioactive Material**

1 Similar to conventional oil and gas production, in unconventional oil and gas production,  
2 radionuclides native to the targeted formation return to the surface with produced water. The  
3 principal radionuclides found in oil and gas produced waters include radium-226 of the uranium-  
4 238 decay series and radium-228 of the thorium-232 decay series ([White, 1992](#)). Levels of  
5 TENORM in produced water are controlled by geologic and geochemical interactions between  
6 injected and formation fluids, and the targeted formation ([Bank, 2011](#)). Mechanisms controlling  
7 NORM mobilization into produced water include (1) the TENORM content of the targeted  
8 formation; (2) factors governing the release of radionuclides, particularly radium, from the  
9 reservoir matrix; and (3) the geochemistry of the produced water ([Choppin, 2007, 2006](#); [Fisher,](#)  
10 [1998](#)).

11 Organic-rich shales and coals are enriched in uranium, thorium, and other trace metals in  
12 concentrations several times above those seen in typical shales or sedimentary rocks ([Diehl et al.,](#)  
13 [2004](#); [USGS, 1997](#); [Wignall and Myers, 1988](#); [Tourtelot, 1979](#); [Vine and Tourtelot, 1970](#)). Unlike  
14 shales and coals, sandstones are generally not organic-rich source rocks themselves. Instead,  
15 hydrocarbons migrate into these formations over long periods of time ([Clark and Veil, 2009](#)). Since  
16 TENORM and organic contents are typically positively correlated due to the original, reduced  
17 depositional environment ([Fertl and Chilingar, 1988](#)), it is unlikely that sandstones would be  
18 enriched in TENORM to the same extent as oil- and gas-bearing shales and coals. Therefore, concern  
19 related to TENORM within produced water is focused on operations targeting shales and coalbeds.

20 Radium is most soluble and mobile in chloride-rich, high-TDS, reducing environments ([Sturchio et](#)  
21 [al., 2001](#); [Zapeczka and Szabo, 1988](#); [Langmuir and Riese, 1985](#)). In formation fluids with high TDS,  
22 calcium, potassium, magnesium, and sodium compete with dissolved radium for sorption sites,  
23 limiting radium sorption onto solids and allowing it to accumulate in solution at higher  
24 concentrations ([Fisher, 1998](#); [Webster et al., 1995](#)). The positive correlation between TDS and  
25 radium is well established and TDS is a useful indicator of radium and TENORM activity within  
26 produced water, especially in lithologically homogenous reservoirs ([Rowan et al., 2011](#); [Sturchio et](#)  
27 [al., 2001](#); [Fisher, 1998](#); [Kraemer and Reid, 1984](#)).

28 Uranium and thorium are poorly soluble under reducing conditions and are therefore more  
29 concentrated in formation solids than in solution ([Fisher, 1998](#); [Kraemer and Reid, 1984](#); [Langmuir](#)  
30 [and Herman, 1980](#)). However, because uranium becomes more soluble in oxidizing environments,  
31 the introduction of relatively oxygen-rich fracturing fluids may promote the temporary  
32 mobilization of uranium during hydraulic fracturing and early flowback. In addition, the physical  
33 act of hydraulic fracturing creates fresh fractures and exposes organic-rich and highly reduced  
34 surfaces from which radionuclides could be released from the rock into formation fluids.

35 Produced water geochemistry determines, in part, the fate of subsurface radionuclides, particularly  
36 radium. Radium may remain in the host mineral or it may be released into formation fluids, where  
37 it can remain in solution as the dissolved  $Ra^{2+}$  ion, be adsorbed onto oxide grain coatings or clay  
38 particles by ion exchange, substitute for other cations during the precipitation of minerals, or form

1 complexes with chloride, sulfate, and carbonate ions ([Rowan et al., 2011](#); [Sturchio et al., 2001](#);  
2 [Langmuir and Riese, 1985](#)). Uranium- and thorium-containing materials with a small grain size, a  
3 large surface-to-volume ratio, and the presence of uranium and thorium near grain surfaces  
4 promote the escape of radium into formation fluids. [Vinson et al. \(2009\)](#) point to alpha decay along  
5 fracture surfaces as a primary control on radium mobilization in crystalline bedrock aquifers.  
6 Radium may also occur in formation fluids due to other processes, such as the decay of dissolved  
7 parent isotopes and adsorption-desorption reactions on formation surfaces ([Sturchio et al., 2001](#)).

8 Preliminary results from fluid-rock interaction studies ([Bank, 2011](#)) indicate that a significant  
9 percentage of uranium in the Marcellus Shale may be subject to mobilization by hydrochloric acid,  
10 which is used as a fracturing fluid additive. Understanding these processes will determine the  
11 extent to which such processes might influence the TENORM content of flowback and produced  
12 water.

### **E.2.6. Organics**

13 Background data on organics in seven formations is given in Table E-9.

**Table E-9. Concentrations of select organic parameters from unconventional shale, a tight formation, and coalbed produced water, presented as: average (minimum–maximum) or *median* (minimum–maximum).**

Parameter	Unit	Shale			Tight Formation	Coal			
		Barnett <sup>a</sup>	Marcellus		Cotton Valley Group <sup>d</sup>	Powder River <sup>e</sup>	Raton <sup>e</sup>	San Juan <sup>e</sup>	Black Warrior <sup>f</sup>
States	n/a	TX	PA <sup>b</sup>	PA, WV <sup>c</sup>	LA, TX	MT, WY	CO, NM	AZ, CO, NM, UT	AL, MS
TOC	mg/L	<b>9.75</b> (6.2–36.2)	160 (1.2–1,530)	<b>89.2</b> (1.2–5680)	198 (184–212)	3.52 (2.07–6.57)	1.74 (0.25–13.00)	2.91 (0.95–9.36)	6.03 (0.00–103.00)
DOC	mg/L	<b>11.2</b> (5.5–65.3)	43 (5–695)	<b>117</b> (3.3–5,960)	-	3.18 (1.09–8.04)	1.26 (0.30–8.54)	3.21 (0.89–11.41)	3.37 (0.53–61.41)
BOD	mg/L	<b>582</b> (101–2,120)	-	<b>141</b> (2.8–12,400)	-	-	-	-	-
Oil and grease	mg/L	<b>163.5</b> (88.2–1,430)	74 (5–802)	<b>16.9</b> (4.7–802)	-	-	9.10 (0.60–17.6)	-	-
Benzene	µg/L	680 (49–5,300)	-	<b>220</b> (5.8–2,000)	-	-	4.7 (BDL–220.0)	149.7 (BDL–500.0)	-
Toluene	µg/L	760 (79–8,100)	-	<b>540</b> (5.1–6,200)	-	-	4.7 (BDL–78.0)	1.7 (BDL–6.2)	-
Ethylbenzene	µg/L	29 (2.2–670)	-	<b>42</b> (7.6–650)	-	-	0.8 (BDL–18.0)	10.5 (BDL–24.0)	-

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Parameter	Unit	Shale			Tight Formation	Coal			
		Barnett <sup>a</sup>	Marcellus		Cotton Valley Group <sup>d</sup>	Powder River <sup>e</sup>	Raton <sup>e</sup>	San Juan <sup>e</sup>	Black Warrior <sup>f</sup>
States	n/a	TX	PA <sup>b</sup>	PA, WV <sup>c</sup>	LA, TX	MT, WY	CO, NM	AZ, CO, NM, UT	AL, MS
Xylenes	µg/L	360 (43–1,400)	-	<b>300</b> (15–6,500)	-	-	9.9 (BDL–190.0)	121.2 (BDL–327.0)	-
Average total BTEX <sup>g</sup>	µg/L	1,829	2,910	1,102	-	-	20.1	283.1	-

n/a, not applicable; -, no value available; BDL, below detection limit. ***Bolded italic*** numbers are medians.

<sup>a</sup> [Hayes and Severin \(2012b\)](#).  $n = 16$ . This data source reported concentrations without presentation of raw data.

<sup>b</sup> [Barbot et al. \(2013\)](#).  $n = 55$ ; no presentation of raw data.

<sup>c</sup> [Hayes \(2009\)](#)  $n = 13$ -67. Concentrations were calculated based on Hayes' raw data. Both flowback and produced water included. Non-detects and contaminated blanks omitted.

<sup>d</sup> [Blondes et al. \(2014\)](#).  $n = 2$ . Concentrations were calculated based on raw data presented in the USGS National Produced Water Database v2.0.

<sup>e</sup> [Dahm et al. \(2011\)](#). Powder River,  $n = 31$ ; Raton,  $n = 40$ ; San Juan,  $n = 20$ . This data source reported concentrations without presentation of raw data.

<sup>f</sup> [DOE \(2014\)](#).  $n = 206$ . Concentrations were calculated based on the authors' raw data.

<sup>g</sup> Average total BTEX was calculated by summing the average/median concentrations of benzene, toluene, ethylbenzene, and xylenes for a unique formation or basin. Minimum to maximum ranges were not calculated due to inaccessible raw data.

1 Several classes of naturally occurring organic chemicals are present in conventional and  
2 unconventional produced waters, with large concentration ranges ([Lee and Neff, 2011](#)). These  
3 organic classes include total organic carbon (TOC); saturated hydrocarbons; BTEX (benzene,  
4 toluene, ethylbenzene, and xylenes); and polyaromatic hydrocarbons (PAHs) (see Table E-9). While  
5 TOC concentrations in produced water are detected at the milligrams to grams per liter level,  
6 concentrations of individual organic compounds are typically detected at the micrograms to  
7 milligrams per liter level.

8 TOC indicates the level of dissolved and undissolved organics in produced water, including non-  
9 volatile and volatile organics ([Acharya et al., 2011](#)). TOC concentrations in conventional produced  
10 water vary widely from less than 0.1 mg/L to more than 11,000 mg/L. Average TOC concentrations  
11 in unconventional produced water range from less than 2.00 mg/L in the Raton CBM basin to  
12 approximately 200 mg/L in the Cotton Valley Group sandstones, although individual measurements  
13 have exceeded 5,000 mg/L in the Marcellus Shale (see Table E-9).

14 Dissolved organic carbon (DOC) is a general indicator of organic loading and is the fraction of  
15 organic carbon available for complexing with metals and supporting microbial growth. DOC values  
16 in unconventional produced water range from less than 1.50 mg/L (average) in the Raton Basin to  
17 more than 115 mg/L (median) in the Marcellus Shale (see Table E-9). Individual DOC  
18 concentrations in the Marcellus Shale produced water approach 6,000 mg/L. For comparison, DOC  
19 levels in fresh water systems are typically below 5 mg/L, while raw wastewater can exceed  
20 50 mg/L ([Katsoyiannis and Samara, 2007](#); [Muylaert et al., 2005](#)).

21 Biochemical oxygen demand (BOD) is a conventional pollutant under the U.S. Clean Water Act. It is  
22 an indirect measure of biodegradable organics in produced water and an estimate of the oxygen  
23 demand on a receiving water. Median BOD levels for Barnett and Marcellus Shales produced water  
24 exceed 30 mg/L, and both reported maximum concentrations exceeding 12,000 mg/L (Table E-9).  
25 In some circumstances wide variation in produced water median BOD levels may be reflective of  
26 flowback reuse in fracturing fluids ([Hayes, 2009](#)).

27 Lastly, BTEX is associated with petroleum. Benzene was found in produced water from several  
28 basins: average produced water benzene concentration from the Barnett Shale was 680 µg/L, from  
29 the Marcellus Shale was 220 µg/L (median), and from the San Juan Basin was 150 µg/L (see Table  
30 E-9). Total BTEX concentrations for conventional produced water vary widely from less than  
31 100 µg/L to nearly 580,000 µg/L. For comparison, average total BTEX concentrations in  
32 unconventional produced water range from 20 µg/L in the Raton Basin to nearly 3,000 µg/L in the  
33 Marcellus play (see Table E-9). From these data, average total BTEX levels in shale produced water  
34 are one to two orders of magnitude higher than those in CBM produced water.

35 In addition to abundant BTEX, a variety of volatile and semi-volatile organic compounds VOCs and  
36 SVOCs have been detected in shale and coalbed produced water. Shale produced water contains  
37 naphthalene, alkylated toluenes, and methylated aromatics in the form of several benzene and  
38 phenol compounds, as shown in Table E-10. Like BTEX, naphthalene, methylated phenols, and  
39 acetophenone are associated with petroleum. Detected shale produced water organics such as

- 1 acetone, 2-butanone, carbon disulfide, and pyridine are potential remnants of chemical additives  
 2 used as friction reducers or industrial solvents ([Hayes, 2009](#)).

**Table E-10. Reported concentrations ( $\mu\text{g/L}$ ) of organic constituents in produced water for two unconventional shale formations, presented as: average (minimum–maximum) or median (minimum–maximum).**

Parameter	Barnett <sup>a</sup>	Marcellus <sup>b</sup>
	States TX	MD, NY, OH, PA, VA, WY
Acetone	145 (27–540)	<b>83</b> (14–5,800)
Carbon disulfide	-	<b>400</b> (19–7,300)
Chloroform	-	28
Isopropylbenzene	35 (0.8–69)	<b>120</b> (86–160)
Naphthalene	238 (4.8–3,100)	<b>195</b> (14–1,400)
Phenolic compounds	<b>119.65</b> (9.3–230)	-
1,2,4-Trimethylbenzene	173 (6.9–1,200)	<b>66.5</b> (7.7–4,000)
1,3,5-Trimethylbenzene	59 (6.4–300)	<b>33</b> (5.2–1,900)
1,2-Diphenylhydrazine	4.2 (0.5–7.8)	-
1,4-Dioxane	6.5 (3.1–12)	-
2-Methylnaphthalene	1,362 (5.4–20,000)	<b>3.4</b> (2–120)
2-Methylphenol	28.3 (5.8–76)	<b>13</b> (11–15)
2,4-Dichlorophenol	(ND–15)	-
2,4-Dimethylphenol	14.5 (8.3–21)	12
3-Methylphenol and 4-Methylphenol	41 (7.8–100)	<b>11.5</b> (0.35–16)
Acetophenone	(ND–4.6)	<b>13</b> (10–22)
Benzidine	(ND–35)	-
Benzo(a)anthracene	(ND–17.0)	-
Benzo(a)pyrene	(ND–130.0)	6.7
Benzo(b)fluoranthene	42.2 (0.5–84.0)	10
Benzo(g,h,i)perylene	42.3 (0.7–84.0)	6.9
Benzo(k)fluoranthene	32.8 (0.6–65.0)	5.9
Benzyl alcohol	81.5 (14.0–200)	<b>41</b> (17–750)
Bis(2-Ethylhexyl) phthalate	210 (4.8–490)	<b>20</b> (9.6–870)
Butyl benzyl phthalate	34.3 (1.9–110)	-

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Parameter	Barnett <sup>a</sup>	Marcellus <sup>b</sup>
States	TX	MD, NY, OH, PA, VA, WY
Chrysene	120 (0.57–240)	-
Di-n-octyl phthalate	(ND–270)	15
Di-n-butyl phthalate	41 (1.5–120)	<b>14</b> (11–130)
Dibenz(a,h)anthracene	77 (3.2–150)	<b>3.2</b> (2.3–11)
Diphenylamine	5.3 (0.6–10.0)	-
Fluoranthene	(ND–0.18)	6.1
Fluorene	0.8 (0.46–1.3)	8.4
Indeno(1,2,3-cd)pyrene	71 (2.9–140)	<b>3.1</b> (2.4–9.5)
N-Nitrosodiphenylamine	8.9 (7.8–10)	2.7
N-Nitrosomethylethylamine	(ND–410)	-
Phenanthrene	107 (0.52–1,400)	<b>9.75</b> (3–22)
Phenol	63 (17–93)	<b>10</b> (2.4–21)
Pyrene	0.2 (ND–0.18)	13
Pyridine	413 (100–670)	<b>250</b> (10–2,600)

-, no value available; ND, not detected.

<sup>a</sup> [Hayes and Severin \(2012b\)](#). *n* = 16. Data from days 1–23 of flowback. This data source reported concentrations without presentation of raw data.

<sup>b</sup> [Hayes \(2009\)](#). *n* = 1–35. Data from days 1–90 of flowback. Concentrations were calculated from Hayes' raw data. Non-detects and contaminated blanks omitted.

1 The organic profile of CBM produced water is characterized by high levels of aromatic and  
2 halogenated compounds compared to other unconventional produced waters ([Sirivedhin and](#)  
3 [Dallbauman, 2004](#)). PAHs and phenols are the most common organic compounds found in coalbed  
4 produced water. Produced water from coalbeds in the Black Warrior Basin mainly contains  
5 phenols, multiple naphthalic PAHs, and various decanoic and decenoic fatty acids (see Table E-11).  
6 CBM-associated organics are also known to include biphenyls, alkyl aromatics, hydroxypyridines,  
7 aromatic amines, and nitrogen-, oxygen-, and sulfur-bearing heterocyclics ([Orem et al., 2014](#);  
8 [Pashin et al., 2014](#); [Benko and Drewes, 2008](#); [Orem et al., 2007](#); [Fisher and Santamaria, 2002](#)).

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**Table E-11. Reported concentrations of organic constituents in 65 samples of produced water from the Black Warrior CBM Basin, presented as average (minimum–maximum).**

Parameter	Number of observations	Concentration (µg/L) <sup>a</sup>
States	-	AL, MS
Benzothiazole	45	0.25 (0.01–3.04)
Caprolactam	10	0.75 (0.02–2.39)
Cyclic octaatomic sulfur	29	1.06 (0.10–9.63)
Dimethyl-naphthalene	39	0.79 (0.01–9.51)
Diethyl phthalate	57	0.21 (0.01–2.30)
Dodecanoic acid	30	1.13 (0.67–2.52)
Hexadecanoic acid	50	1.58 (1.17–3.02)
Hexadecenoic acid	25	1.69 (1.13–8.37)
Methyl-biphenyl	18	0.25 (0.01–2.13)
Methyl-naphthalene	52	0.77 (0.01–15.55)
Methyl-quinoline	31	0.96 (0.03–3.75)
Naphthalene	49	0.41 (0.01–6.57)
Octadecanoic acid	32	1.95 (1.62–3.73)
Octadecenoic acid	29	1.87 (1.60–3.47)
Phenol, 2,4-bis(1,1-dimethyl)	21	0.45 (0.01–4.94)
Phenol, 4-(1,1,3,3-tetramethyl)	17	1.65 (0.01–18.34)
Phenolic compounds	-	19.06 (ND–192.00)
Tetradecanoic acid	53	1.51 (0.94–5.32)
Tributyl phosphate	23	0.26 (0.01–2.66)
Trimethyl-naphthalene	23	0.65 (0.01–4.49)
Triphenyl phosphate	6	1.18 (0.01–6.77)

-, no value available.

<sup>a</sup> [DOE \(2014\)](#). Concentrations were calculated based on the authors' raw data.

1 [Hayes \(2009\)](#) characterized the content of Marcellus Shale produced water including organics (see  
2 Table E-10). The author tested for the majority of VOCs and SVOCs, pesticides and PCBs, based on  
3 the recommendation of the Pennsylvania and West Virginia Departments of Environmental  
4 Protection. Only 0.5% of VOCs and 0.03% of SVOCs in the produced water were detected above  
5 1 mg/L. Approximately 96% of VOCs, 98% of SVOCs, and virtually all pesticides and PCBs were at  
6 nondetectable levels.

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### E.2.7. Chemical Reactions

1 Section E.2.7.1 describes general aspects of subsurface chemical reactions that might occur during  
2 hydraulic fracturing operations. Here we augment the discussion by describing subsurface chemical  
3 processes.

#### E.2.7.1. Injected Chemical Processes

4 Hydraulic fracturing injects relatively oxygenated fluids into a reducing environment, which may  
5 mobilize trace or major constituents into solution. Injection of oxygenated fluids may lead to  
6 short-term changes in the subsurface redox state, as conditions may shift from reducing to  
7 oxidizing. The chemical environment in hydrocarbon-rich unconventional reservoirs, such as black  
8 shales, is generally reducing, as evidenced by the presence of pyrite and methane ([Engle and  
9 Rowan, 2014](#); [Dresel and Rose, 2010](#)). For black shales, reducing conditions are a product of  
10 original accumulations of organic matter whose decay depleted oxygen to create rich organic  
11 sediments within oil- and gas-producing formations ([Tourtelot, 1979](#); [Vine and Tourtelot, 1970](#)).  
12 Yet reactions resulting from temporary redox shifts are likely to be less important than those  
13 resulting from other longer-term physical and geochemical processes. Temporary subsurface redox  
14 shifts may be due to the short timeframe for fluid injection (a few days to a few weeks) and the use  
15 of oxygen scavengers to prevent downhole equipment corrosion.

16 Hydraulic fracturing fluid injection introduces novel chemicals into the subsurface.<sup>1</sup> As such, the  
17 geochemistry of injected and native fluids will not be in equilibrium. Over the course of days to  
18 months, a complex series of reactions will equilibrate disparate fluid chemistries. The evolution of  
19 flowback and produced water geochemistry are dependent upon the exposure of formation solids  
20 and fluids to novel chemicals within hydraulic fracturing fluid. Chemical additives interact with  
21 reservoir solids and either mobilize constituents or themselves become adsorbed to solids. Such  
22 additives include metallic salts, elemental complexes, salts of organic acids, organometallics, and  
23 other metal compounds ([Montgomery, 2013](#); [House of Representatives, 2011](#)).

24 The salts, elemental complexes, organic acids, organometallics, and other metal-containing  
25 compounds may interact with metals and metalloids in the target formation through processes  
26 such as ion exchange, adsorption, desorption, chelation, and complexation. For instance, natural  
27 organic ligands (e.g., citrate) are molecules that can form coordination compounds with heavy  
28 metals such as cadmium, copper, and lead ([Martinez and McBride, 2001](#); [Stumm and Morgan, 1981](#);  
29 [Bloomfield et al., 1976](#)). Citrate-bearing compounds are used in hydraulic fracturing fluids as  
30 surfactants, iron control agents, and biocides. Studies of the additives' interactions with formation  
31 solids at concentrations representative of hydraulic fracturing fluids are lacking.

32 Furthermore, pH will likely play a role in the nature and extent of these processes, as the low pH of  
33 hydraulic fracturing fluids may mobilize trace constituents. The pH of injected fluids may differ  
34 from existing subsurface conditions due to the use of dilute acids (e.g., hydrochloric or acetic) used  
35 for cleaning perforations and fractures during hydraulic fracturing treatments ([Montgomery, 2013](#);

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<sup>1</sup> For more information on chemical additive usage, refer to Chapter 5 (Chemical Mixing).

1 [GWPC and ALL Consulting, 2009](#)). Metals within formation solids may be released through the  
2 dissolution of acid-soluble phases such as iron and manganese oxides or hydroxides ([Yang et al.,](#)  
3 [2009](#); [Kashem et al., 2007](#); [Filgueiras et al., 2002](#)). Thus, the pH of hydraulic fracturing fluids, or  
4 changes in system pH that may occur as fluid recovery begins, may influence which metals and  
5 metalloids are likely to be retained within the formation and which may be recovered in flowback.  
6 Ultimately, more research is needed to fully understand how the injection of hydraulic fracturing  
7 fluids affects subsurface geochemistry and resultant flowback and produced water chemistry.

### **E.2.8. Microbial Community Processes and Content**

8 By design, hydraulic fracturing releases hydrocarbons and other reduced mineral species from  
9 freshly fractured shale, sandstone, and coal, resulting in saltier in situ fluids, the release of  
10 formation solids, and increased interconnected fracture networks with rich colonization surfaces  
11 that are ideal for microbial growth ([Wuchter et al., 2013](#); [Curtis, 2002](#)). Depending upon the  
12 formation, microorganisms may be native to the subsurface and/or introduced from non-sterile  
13 equipment and fracturing fluids. Additionally, microorganisms compete for novel organics in the  
14 form of chemical additives ([Wuchter et al., 2013](#); [Arthur et al., 2009](#)). Since large portions of  
15 hydraulic fracturing fluid can remain emplaced in the targeted formation, long-term microbial  
16 activity is supported through these novel carbon and energy resources ([Orem et al., 2014](#); [Murali](#)  
17 [Mohan et al., 2013a](#); [Struchtemeyer and Elshahed, 2012](#); [Bottero et al., 2010](#)). Such physical and  
18 chemical changes to the environment at depth stimulate microbial activity and influence flowback  
19 and produced water content in important ways.

20 Several studies characterizing produced water from unconventional formations (i.e., the Barnett,  
21 Marcellus, Utica, and Antrim Shales) indicate that taxa with recurring physiologies compose shale  
22 flowback and produced water microbial communities ([Murali Mohan et al., 2013b](#); [Wuchter et al.,](#)  
23 [2013](#)). Such physiologies include sulfur cyclers (e.g., sulfidogens: sulfur , sulfate , and thiosulfate  
24 reducers); fermenters; acetogens; hydrocarbon oxidizers; methanogens; and iron, manganese, and  
25 nitrate reducers ([Davis et al., 2012](#)).

26 Based on their physiologies, microorganisms cycle substrates at depth by mobilizing or  
27 sequestering constituents in and out of solution. Mobilization can occur through biomethylation,  
28 complexation, and leaching. Sequestration can occur through intracellular sequestration,  
29 precipitation, and sorption to biomass.

30 The extent to which constituents are mobilized or sequestered depends upon the prevailing  
31 geochemical environment after hydraulic fracturing and through production. Significant  
32 environmental factors that influence the extent of microbially mediated reactions are increases in  
33 ionic content (i.e., salinity, conductivity, total nitrogen, bromide, iron, and potassium); decreases in  
34 acidity, and organic and inorganic carbon; the availability of diverse electron acceptors and donors;  
35 and the availability of sulfur-containing compounds ([Cluff et al., 2014](#); [Murali Mohan et al., 2013b](#);  
36 [Davis et al., 2012](#)). Examples follow that illustrate how subsurface microbial activity influences the  
37 content of produced water.

1 Under prevailing anaerobic and reducing conditions, microorganisms can mobilize or sequester  
2 metals found in unconventional produced water ([Gadd, 2004](#)). Microbial enzymatic reduction  
3 carried out by chromium-, iron-, manganese-, and uranium-reducing bacteria can both mobilize and  
4 sequester metals ([Vanengelen et al., 2008](#); [García et al., 2004](#); [Mata et al., 2002](#); [Gauthier et al.,](#)  
5 [1992](#); [Myers and Nealson, 1988](#); [Lovley and Phillips, 1986](#)). For instance, iron and manganese  
6 species go into solution when reduced, while chromium and uranium species precipitate when  
7 reduced ([Gadd, 2004](#); [Newman, 2001](#); [Ahmann et al., 1994](#)).

8 Metals can also be microbially solubilized by complexing with extracellular metabolites,  
9 siderophores (metal-chelating compounds), and microbially generated bioligands (e.g., organic  
10 acids) ([Glorius et al., 2008](#); [Francis, 2007](#); [Gadd, 2004](#); [Hernlem et al., 1999](#)). For example,  
11 *Pseudomonas* spp. secrete acids that act as bioligands to form complexes with uranium(VI) ([Glorius](#)  
12 [et al., 2008](#)).

13 Many sulfur-cycling taxa have been found in hydraulic fracturing flowback and produced water  
14 communities ([Murali Mohan et al., 2013b](#); [Mohan et al., 2011](#)). Immediately following injection,  
15 microbial sulfate reduction is stimulated by diluting high-salinity formation waters with fresh  
16 water (high salinities inhibit sulfate reduction). Microbial sulfate reduction oxidizes organic matter  
17 and decreases aqueous sulfate concentrations, thereby increasing the solubility of barium ([Cheung](#)  
18 [et al., 2010](#); [Lovley and Chapelle, 1995](#)).

19 Sulfidogens also reduce sulfate, as well as elemental sulfur and other sulfur species (e.g.,  
20 thiosulfate) prevalent in the subsurface, contributing to biogenic sulfide or hydrogen sulfide gas in  
21 produced water ([Alain et al., 2002](#); [Ravot et al., 1997](#)). Sulfide can also sequester metals in sulfide  
22 phases ([Ravot et al., 1997](#); [Lovley and Chapelle, 1995](#)). Sources of sulfide also include formation  
23 solids (e.g., pyrite in shale) and remnants of drilling muds (e.g., barite and sulfonates), or other  
24 electron donor sources ([Davis et al., 2012](#); [Kim et al., 2010](#); [Collado et al., 2009](#); [Grabowski et al.,](#)  
25 [2005](#)).

26 Additionally, anaerobic hydrocarbon oxidizers associated with shale produced water can readily  
27 degrade simple and complex carbon compounds across a considerable salinity and redox range  
28 ([Murali Mohan et al., 2013b](#); [Fichter et al., 2012](#); [Timmis, 2010](#); [Lalucat et al., 2006](#); [Yakimov et al.,](#)  
29 [2005](#); [McGowan et al., 2004](#); [Hedlund et al., 2001](#); [Cayol et al., 1994](#); [Gauthier et al., 1992](#); [Zeikus et](#)  
30 [al., 1983](#)).

31 Lastly, microbial fermentation produces organic acids, alcohols, and gases under anaerobic  
32 conditions, as is the case during methanogenesis. Some nitrogen-cycling genera have been  
33 identified in unconventional shale gas systems. These include genera involved in nitrate reduction  
34 and denitrification ([Kim et al., 2010](#); [Yoshizawa et al., 2010](#); [Yoshizawa et al., 2009](#); [Lalucat et al.,](#)  
35 [2006](#)). These genera likely couple sugar, organic carbon, and sulfur species oxidation to nitrate  
36 reduction and denitrification processes.

1 Consequently, using a variety of recurring physiologies, microorganisms mobilize and sequester  
2 constituents in and out of solution to influence the content of flowback and produced water in  
3 important ways.

### E.3. Produced Water Content Spatial Trends

#### E.3.1. Variability between Plays of the Same Rock Type

##### E.3.1.1. Shale Formation Variability

4 The content of shale produced water varies geographically, as shown by data from four formations  
5 (the Bakken, Barnett, Fayetteville, and Marcellus Shales; see Table E-2, Table E-4, Table E-6, Table  
6 E-9, Table E-10). For several constituents, variability between shale formations is common. The  
7 average/median TDS concentrations in the Marcellus (87,800 to 106,390 mg/L) and Bakken  
8 (196,000 mg/L) Shales are one order of magnitude greater than the average TDS concentrations  
9 reported for the Barnett and Fayetteville Shales (see Table E-2). As Fayetteville produced water  
10 contains the lowest reported average TDS concentration (13,290 mg/L), average concentrations for  
11 many inorganics (i.e., bromide, calcium, chloride, magnesium, sodium, and strontium) that  
12 contribute to dissolved solids loads are the lowest compared to average concentrations for the  
13 same inorganics in Bakken, Barnett, and Marcellus produced water (see Table E-4 and Table E-6).  
14 Average concentrations for metals reported within Bakken and Marcellus produced water are also  
15 higher than those within the Barnett or Fayetteville formations (see Table E-6).

16 Additionally, Marcellus produced water is enriched in barium (average concentration of 2,224 mg/l  
17 in [Barbot et al. \(2013\)](#) or median calculated from [Hayes \(2009\)](#) of 542.5 mg/L) and strontium  
18 (average concentration of 1,695 mg/L ([Barbot et al., 2013](#)) or median calculated from [Hayes](#)  
19 [\(2009\)](#) of 1,240 mg/L) by one to three orders of magnitude compared to Bakken, Barnett, and  
20 Fayetteville produced water (see Table E-6). Subsequently, radionuclide variability expressed as  
21 isotopic ratios (e.g., radium-228/radium-226, strontium-87/strontium-86) are being used to  
22 determine the reservoir source for produced water ([Chapman et al., 2012](#); [Rowan et al., 2011](#);  
23 [Blauch et al., 2009](#)). Lastly, Barnett and Bakken produced waters are enriched in sulfate.

24 Although organic data are limited, average BTEX concentrations are higher in Marcellus compared  
25 to Barnett produced water by one order of magnitude, whereas concentrations of benzene alone  
26 are marginally higher in Barnett compared to Marcellus produced water (see Table E-9 and Table  
27 E-10).

##### E.3.1.2. Tight Formation Variability

28 The average concentrations for various constituents in tight formation produced water vary  
29 geographically between sandstone formations (the Cotton Valley Group, Devonian sandstone, and  
30 the Mesaverde and Oswego), as shown in Table E-2, Table E-4, and Table E-6. The average TDS  
31 concentrations in the Devonian sandstone (235,125 mg/L) and Cotton Valley Group  
32 (164,683 mg/L) are one to two orders of magnitude greater than the average TDS concentrations  
33 reported for the Mesaverde (15,802 mg/L) and Oswego Formations (73,082 mg/L) (see Table E-2).

1 Mesaverde produced water also contained the lowest average concentrations for many of the  
2 inorganic components of TDS (i.e., calcium, chloride, iron, magnesium, and sodium; see Table E-4  
3 and Table E-6).

4 Little variability was reported in pH between these four tight formations (see Table E-2).  
5 Mesaverde produced water was enriched in sulfate, with an average concentration of 837 mg/L  
6 (see Table E-4), whereas Devonian produced water was enriched in barium, which had an average  
7 concentration of 1,488 mg/L (see Table E-6).

### **E.3.1.3. Coalbed Variability**

8 Geochemical analysis showed that the Powder River Basin is predominately characterized by  
9 bicarbonate water types with a large intrusion of sodium-type waters across a large range of  
10 magnesium and calcium concentrations ([Dahm et al., 2011](#)).<sup>1</sup> In contrast, the Raton Basin is typified  
11 by sodium-type waters with low calcium and magnesium concentrations. A combination of Powder  
12 River and Raton produced water compositional characteristics typifies the San Juan Basin ([Dahm et](#)  
13 [al., 2011](#)). Lastly, Black Warrior Basin produced water is differentiated based upon its sodium  
14 bicarbonate- or sodium chloride-type waters ([DOE, 2014](#); [Pashin et al., 2014](#)).

15 Regional variability is observed in average produced water concentrations for various constituents  
16 of four CBM basins (Powder River, Raton, San Juan, and Black Warrior; see Table E-3, Table E-5,  
17 Table E-7, Table E-9, and Table E-11), but particularly between produced water of the Black  
18 Warrior Basin and the others. As the average TDS concentration in Black Warrior Basin produced  
19 water (14,319 mg/L) is one to two orders of magnitude higher than that of the other three  
20 presented in Table E-3, average concentrations for TDS contributing ions (i.e., calcium, chloride,  
21 and sodium) were also higher than in the Powder River, Raton, and San Juan Basins. These high  
22 levels follow from the marine depositional environment of the Black Warrior Basin ([Horsey, 1981](#)).

23 Powder River Basin produced water has the lowest average TDS concentration (997 mg/L), which  
24 is consistent with [Dahm et al. \(2011\)](#) reporting that nearly a quarter of all the produced water  
25 sampled from the Powder River Basin meets the U.S. drinking water secondary standard for TDS  
26 (less than 500 mg/L).<sup>2</sup> In addition, the Black Warrior Basin appears to be slightly enriched in  
27 barium, compared to the other three CBM basins (see Table E-5). Lastly, the three western CBM  
28 basins (Powder River, Raton, and San Juan) are much more alkaline and enriched in bicarbonate  
29 than their eastern counterpart (the Black Warrior Basin; see Table E-3).

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<sup>1</sup> Water is classified as a “type” if the dominant dissolved ion is greater than 50% of the total. A sodium-type water contains more than 50% of the cation milliequivalents (mEq) as sodium. Similarly, a sodium-bicarbonate water contains 50% of the cation mEq as sodium, and 50% of the anion mEq as bicarbonate ([USGS, 2002](#)).

<sup>2</sup> MCL refers to the highest level of a contaminant that is allowed in drinking water. MCLs are enforceable standards. These include primary MCLs for barium, cadmium, chromium, lead, mercury, and selenium. National Secondary Drinking Water Regulations (NSDWRs or secondary standards) are non-enforceable guidelines regulating contaminants that may cause cosmetic effects (such as skin or tooth discoloration) or aesthetic effects (such as taste, odor, or color) in drinking water. Secondary MCLs are recommended for aluminum, chloride, copper, iron, manganese, pH, silver, sulfate, TDS, and others. See <http://water.epa.gov/drink/contaminants/index.cfm#Primary> for more information.

1 Average concentrations of benzene, ethylbenzene, and xylenes are higher in San Juan compared to  
2 Raton produced water by two orders of magnitude, whereas concentrations of toluene are  
3 marginally higher in Raton compared to San Juan produced water (see Table E-9).

### E.3.2. Local Variability

4 Spatial variability of produced water content frequently exists within a single producing formation.  
5 For instance, Marcellus Shale barium levels increase along a southwest to northeast transect  
6 ([Barbot et al., 2013](#)). Additionally, produced water from the northern and southern portions of the  
7 San Juan Basin differ in TDS, due to ground water recharge in the northern basin leading to higher  
8 chloride concentrations than in the southern portion ([Dahm et al., 2011](#); [Van Voast, 2003](#)).

9 Spatial variability of produced water content also exists at a local level due to the stratigraphy  
10 surrounding the producing formation. For example, deep saline aquifers, if present in the over- or  
11 underlying strata, may over geologic time encroach upon shales, coals, and sandstones via fluid  
12 intrusion processes ([Blauch et al., 2009](#)). Evidence of deep brine migration from adjacent strata into  
13 shallow aquifers via natural faults and fractures has been noted previously in the Michigan Basin  
14 and the Marcellus Shale ([Vengosh et al., 2014](#); [Warner et al., 2012](#); [Weaver et al., 1995](#)). By  
15 extension, in situ hydraulic connectivity, which is stimulated by design during hydraulic fracturing,  
16 may lead to the migration of brine-associated constituents in under- and overlying strata into  
17 producing formations, as discussed in Chapter 6.

18 As hydrocarbon source rocks often form repeating sedimentary sequences, contact between these  
19 layers presents opportunities for an exchange of organics and inorganics ([Fredrickson and Balkwill,](#)  
20 [2006](#); [U.S. EPA, 2004](#)). For instance, diffusion of carbon sources and electron donors occurs at  
21 subsurface shale-sandstone interfaces, suggesting a stratigraphic role in the exchange of  
22 constituents between formations ([Fredrickson and Balkwill, 2006](#)).

## E.4. Example Calculation for Roadway Transport

23 This section provides background information for the roadway transport calculation appearing in  
24 Chapter 7.

### E.4.1. Estimation of Transport Distance

25 In a study of wastewater management for the Marcellus Shale, [Rahm et al. \(2013\)](#) used data  
26 reported to the Pennsylvania Department of Environmental Protection (PA DEP) to estimate the  
27 average distance wastewater was transported. For the period from 2008 to 2010, the distance  
28 transported was approximately 100 km, but it was reduced by 30% for 2011. The reduction was  
29 attributed to increased treatment infrastructure in Lycoming County, an area of intensive hydraulic  
30 fracturing operations in northeastern Pennsylvania. For the part of Pennsylvania within the  
31 Susquehanna River Basin, [Gilmore et al. \(2013\)](#) estimated the likely transport distances for drilling  
32 waste to landfills (256 km or 159 mi); produced water to disposal wells (388 km or 241 mi); and  
33 commercial wastewater treatment plants (CWTPs) (158 km or 98 mi). These distances are longer

1 than the values from [Rahm et al. \(2013\)](#), in part, because wells in the Susquehanna Basin are  
 2 further to the east of Ohio disposal wells and some CWTPs.

#### E.4.2. Estimation of Wastewater Volumes

3 In an example water balance calculation, [Gilmore et al. \(2013\)](#) used 380,000 gal of flowback as the  
 4 volume transported to CWTPs, 450,000 gal of flowback transported to injection wells, and 130,000  
 5 gal of un-reusable treated water also transported to injection wells for a total estimated wastewater  
 6 volume of 960,000 gal per well.

#### E.4.3. Estimation of Roadway Accidents

7 The U.S. Department of Transportation (DOT) published statistics on roadway accidents ([U.S.  
 8 Department of Transportation, 2012](#)) which indicate that the combined total of combination truck  
 9 crashes in 2012 was 179,736, or 110 per 100 million vehicle miles (1.77 million km) (see Table  
 10 E-12). As an indicator of the uncertainty of these data, DOT reported 122,240 large truck crashes  
 11 from a differing set of databases (see Table E-13), with a rate of 75 per 100 million vehicle miles,  
 12 which is 68% of the number of combination truck crashes.

**Table E-12. Combination truck crashes in 2012 for the 2,469,094 registered combination trucks, which traveled 163,458 million miles (U.S. Department of Transportation, 2012).<sup>a</sup>**

Type of crash	Combination trucks involved in crashes	Rates per 100 million vehicle miles traveled by combination trucks
Property damage only	135,000	82.8
Injury	42,000	25.5
Fatal	2,736	1.74
Total	179,736	110

<sup>a</sup> A combination truck is defined as a truck tractor pulling any number of trailers ([U.S. Department of Transportation, 2012](#)).

**Table E-13. Large truck crashes in 2012 (U.S. Department of Transportation, 2012).<sup>a</sup>**

Type of crash	Total crashes	Large trucks with cargo tanks	
		Number	Percentage
Towaway crashes	72,644	4,364	6.0%
Injury	45,794	3,245	7.1%
Fatal	3,802	360	9.5%
Totals	122,240	7,969	6.5%

<sup>a</sup> A large truck is defined as a truck with a gross vehicle weight rating greater than 10,000 pounds ([U.S. Department of Transportation, 2012](#)).

#### E.4.4. Estimation of Material Release Rates in Crashes

1 Estimates ranging from 5.6% to 36% have been made for the probability of material releases from  
 2 crashed trucks. [Craft \(2004\)](#) used data from three databases to estimate the probability of spills in  
 3 fatality accidents at 36%, which may overestimate the probability for all types of accidents ([Rozell  
 4 and Reaven, 2012](#)).<sup>1</sup> The [U.S. Department of Transportation \(2012\)](#) provides estimates of  
 5 hazardous materials releases from large truck crashes. For all types of hazardous materials carried,  
 6 408 of 2,903 crashes, or 14%, were known to have hazardous materials releases. The occurrence of  
 7 a release was unknown for 18% of the crashes. These crashes were not distinguished by truck type,  
 8 so they likely overestimated the number of tanker crashes. [Harwood et al. \(1993\)](#) used accident  
 9 data from three states (California, Illinois, and Michigan) to develop hazardous materials release  
 10 rate estimates for different types of roadways, accidents, and settings (urban or rural). For  
 11 roadways in rural settings the probability of release ranged from 8.1% to 9.0%, while in urban  
 12 settings the probability ranged from 5.6% to 6.9%.

#### E.4.5. Estimation of Volume Released in Accidents

13 Based on the estimated volume (960,000 gal (3.63 million L) per well) and disposal distances used  
 14 by [Rahm et al. \(2013\)](#) and [Gilmore et al. \(2013\)](#), and an assumed 20,000 L (5,300 gal)-containing  
 15 truck ([Gilmore et al., 2013](#)), the total travel distance by trucks ranges from 9,620 miles (14,900 km)  
 16 to 17,760 miles (28,570 km) per well (see Table E-14).

<sup>1</sup> The three databases were the Trucks Involved in Fatal Accidents developed by the Center for National Truck Statistics at the University of Michigan, the National Automotive Sampling System's General Estimates System (GES) produced by the National Highway Transportation Safety Agency, and the Motor Carrier Management Information System (MCMIS) Crash File produced by the Federal Motor Carrier Safety Administration.

**Table E-14. Estimate of total truck-travel miles per well in the Susquehanna River Basin based on the transport analysis performed by Gilmore et al. (2013).**

Action	Waste per well (million gal)	Trucks (20 m <sup>3</sup> /truck)	Miles traveled per truck	Total miles traveled (per well)	Material release rate bounds			
					5.6%		36%	
					Crashes per 100 million miles			
					75	110	75	110
<b><i>Gilmore et al. (2013) distance estimates</i></b>								
Produced water to CWTP	0.38	72	26.9	1,937				
Produced water to disposal well	0.45	85	147	12,495				
CWTP effluent to disposal well	0.13	25	133	3,325				
Total	0.96	182		17,757	3	4	18	27
<b><i>Rahm et al. (2013) distance estimates</i></b>								
Transport 100 km	0.96	182	62.1	11,300	2	3	12	17
Transport 70 km	0.96	182	43.5	9,620	1	2	8	12

- 1 The Susquehanna River Basin Commission reported 1,928 well pads permitted within the basin  
2 ([SRBC, 2012](#)). Assuming two wells per pad, the total distance traveled to haul hydraulic fracturing  
3 wastewater is 68.4 million miles (110 million km).
- 4 Combining these data with the DOT crash data gives an estimated 76 crashes per year using the  
5 combination truck crash rate or 52 per year using the DOT large truck crash rate. Based on the  
6 various assumptions of travel distances, crash rates, and estimated minimum and maximum  
7 material release rates, the number of crashes with releases ranges from 1 to 27 (see Table E-14).
- 8 Several limitations are inherent in this analysis, including differing rural road accident rates and  
9 highway rates, differing wastewater endpoints, and differing amounts of produced water transport.  
10 Further, the estimates present an upper bound on impacts, because not all releases of wastewater  
11 would reach or impact drinking water resources.

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## Appendix F

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# Wastewater Treatment and Waste Disposal Supplemental Information

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## Appendix F. Wastewater Treatment and Waste Disposal Supplemental Information

1 This appendix provides additional information for context and background to support the  
2 discussions of hydraulic fracturing wastewater management and treatment in Chapter 8 of the  
3 Hydraulic Fracturing Drinking Water Assessment. Information in this appendix includes: estimates  
4 compiled for several states for volumes of wastewater generated in regions where hydraulic  
5 fracturing is occurring; an overview of the technologies that can be used to treat hydraulic  
6 fracturing wastewater; calculations of estimated treatment process effluent concentrations for  
7 example constituents; a description of the different discharge options for centralized waste  
8 treatment plants; and the water quality needed for wastewater to be reused for hydraulic  
9 fracturing. Discussion is also provided on difficulties that can arise during treatment of hydraulic  
10 fracturing wastewaters: the potential impacts of hydraulic fracturing wastewater on biological  
11 treatment processes; and an overview of the formation of disinfection byproducts.

### F.1. Estimates of Wastewater Production in Regions where Hydraulic Fracturing is Occurring

12 Table F-1 presents estimated wastewater volumes for several states in areas with hydraulic  
13 fracturing activity. These data were compiled from production data available on state databases  
14 and were tabulated by year. For California, data were compiled for Kern County, where about 95%  
15 of hydraulic fracturing is taking place ([CCST, 2015](#)). Production records from Colorado, Utah, and  
16 Wyoming include the producing formation for each well reported; data from these states were  
17 filtered to select data from formations indicated in the literature as targets for hydraulic fracturing.  
18 Data presented for these three states include statewide estimates as well as estimates for selected  
19 basins. Data from New Mexico are available from the states in files for three basins as well as for the  
20 state; these data were not filtered further.

21 Results in Table F-1 illustrate some of the challenges associated with obtaining estimates of  
22 hydraulic fracturing wastewater volumes, especially using publicly available data. Some of the  
23 values likely include reported values from conventional wells (wells that may not be hydraulically  
24 fractured, and are typically not subject to modern, high volume hydraulic fracturing). For example,  
25 the well counts for California, Colorado, Utah, and Wyoming were in the thousands or tens of  
26 thousands at least as early as 2000, several years before the surge of modern hydraulic fracturing  
27 began in the mid-2000s. The data used for California were from Kern County but are not specific to  
28 hydraulic fracturing activity. Where producing formations are provided, the accuracy of the  
29 estimates will depend upon correct selection of hydraulically fractured formations. Thus, both  
30 underestimation and overestimation may be possible because of a lack of clear indication of which  
31 wells were hydraulically fractured.

**Table F-1. Estimated volumes (millions of gallons) of wastewater based on state data for selected years and numbers of wells producing fluid.**

State	Basin	Principal lithologies	Data type	2000	2004	2008	2010	2011	2012	2013	2014	Comments
California	San Joaquin <sup>a</sup>	Shale, unconsolidated sands	Produced water	46,000	48,000	58,000	65,000	71,000	75,000	74,000	-	Data from CA Department of Conservation, Oil and Gas Division. <sup>a</sup> Produced water data compiled for Kern County. Data may also represent contributions from production without hydraulic fracturing.
			Wells	33,695	39,088	46,519	49,201	51,031	51,567	52,763	-	
Colorado	All basins with hydraulically fractured formations	-	Produced water	7,300	11,000	21,000	14,000	12,000	12,000	7,700	-	Data from CO Oil and Gas Conservation Commission. <sup>b</sup> Produced water includes flowback. Data filtered for formations indicated in literature as undergoing hydraulic fracturing and matched to corresponding basins. Example counties selected for presentation as well as estimated state total.
			Wells	11,264	14,934	28,282	33,929	35,999	38,371	37,618	-	
	Denver	Sandstone, shale	Produced water	140	160	170	160	160	150	110	-	
			Wells	1,829	1,511	1,277	1,204	1,193	1,131	1,072	-	
	Piceance	Sandstone	Produced water	3,500	5,800	9,300	6,900	6,500	6,800	4,300	-	
			Wells	1,134	2,478	6,486	9,105	10,057	10,868	10,954	-	

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State	Basin	Principal lithologies	Data type	2000	2004	2008	2010	2011	2012	2013	2014	Comments	
Colorado, cont.	Raton	Coalbed methane	Produced water	2,400	4,100	8,900	4,300	3,200	2,700	2,100	-		
			Wells	681	1,634	2,795	2,734	2,778	2,710	2,545	-		
	San Juan	Coalbed methane	Produced water	1,000	1,100	1,300	2,000	1,200	1,100	650	-		
			Wells	1,183	1,605	1,975	2,220	2,308	2,328	2,333	-		
New Mexico	Permian	Shale, sandstone	Produced water	-	-	-	-	-	31,000	31,000	20,000	Data from New Mexico Oil Conservation Division. <sup>c</sup> Data provided by the state by basin and for the entire state. Unclear how much contribution from production without hydraulic fracturing. Produced water includes flowback.	
			Wells	-	-	-	-	-	29,839	30,386	30,287		
	Raton	Coalbed methane	Produced water	-	-	-	-	-	510	540	310		
			Wells	-	-	-	-	-	1,495	1,502	1,526		
	San Juan	Coalbed methane	Produced water	-	-	-	-	-	1,700	2,000	1,100		
			Wells	-	-	-	-	-	22,492	22,349	22,076		
	Total	-		Produced water	-	-	-	-	-	33,000	34,000	22,000	
				Wells	-	-	-	-	-	53,826	54,237	53,889	

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State	Basin	Principal lithologies	Data type	2000	2004	2008	2010	2011	2012	2013	2014	Comments	
Utah	All basins with hydraulically fractured formations	-	Produced water	1,200	1,200	2,300	2,400	2,700	2,900	3,400	2,800	Data from State of Utah Oil and Gas Program. <sup>d</sup> Produced water includes flowback. Data filtered by formation indicated in the literature as hydraulically fractured and matched to basins. Data presented for selected basins as well as for all formations likely to be hydraulically fractured.	
			Wells	3,080	4,377	7,409	8,432	9,101	10,075	10,661	10,900		
	Kaiparowits/ Uinta	Coalbed methane	Produced water	860	740	1,300	1,400	1,800	2,000	2,400	1,900		
			Wells	1,718	2,517	3,761	4,329	4,838	5,538	6,046	6,334		
	San Juan/ Uinta	Coalbed methane	Produced water	2	49	350	270	240	230	190	120		
			Wells	62	223	910	933	959	951	867	870		
	Uinta	Shale/sandstone	Produced water	350	420	560	680	700	640	830	790		
			Wells	1,067	1,396	2,282	2,745	2,888	3,115	3,257	3,223		
	Wyoming	All basins with hydraulically fractured formations	-	Produced water	1,300	1,400	1,300	1,500	1,600	1,700	1,600	1,800	Data from Wyoming Oil and Gas Conservation Commission. <sup>e</sup> Produced water may include flowback. Data filtered by formation indicated in the literature as hydraulically fractured and matched to basins. Data presented for selected basins as well as for all formations likely to be hydraulically fractured.

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State	Basin	Principal lithologies	Data type	2000	2004	2008	2010	2011	2012	2013	2014	Comments
Wyoming, cont.			Wells	3,470	3,378	3,585	3,620	3,728	3,843	4,030	4,213	
	Big Horn	Sandstone	Produced water	380	350	350	380	430	440	420	440	
			Wells	365	359	387	397	412	414	407	403	
	Denver	Sandstone	Produced water	54	44	49	59	76	90	97	170	
			Wells	142	118	124	140	167	204	230	278	
	Green River	Sandstone/shale	Produced water	0	1	2	8	5	5	9	15	
			Wells	44	44	60	67	67	59	64	67	
	Powder River	Coalbed methane	Produced water	690	630	620	660	700	840	970	1,100	
			Wells	1,953	1,900	2,001	2,028	2,119	2,207	2,352	2,565	
	Wind River/ Powder River	Sandstone/shale	Produced water	130	330	330	400	420	290	110	41	
			Wells	966	957	1,013	988	963	959	977	900	

<sup>a</sup> California Department of Conservation, Oil and Gas Division. Oil & Gas – Online Data. Monthly Production and Injection Databases: [ftp://ftp.consrv.ca.gov/pub/oil/new\\_database\\_format/](ftp://ftp.consrv.ca.gov/pub/oil/new_database_format/).

<sup>b</sup> Colorado Oil and Gas Conservation Commission. Data: Downloads: Production Data: <http://cogcc.state.co.us/data2.html#/downloads>.

<sup>c</sup> New Mexico Oil Conservation Division. Production Data. Production Summaries: All Wells Data: [http://gotech.nmt.edu/gotech/Petroleum\\_Data/allwells.aspx](http://gotech.nmt.edu/gotech/Petroleum_Data/allwells.aspx).

<sup>d</sup> Utah Department of Natural Resources. Division of Oil, Gas, and Mining. Data Research Center. Database Download Files: [http://oilgas.ogm.utah.gov/Data\\_Center/DataCenter.cfm#production](http://oilgas.ogm.utah.gov/Data_Center/DataCenter.cfm#production).

<sup>e</sup> Wyoming Oil and Gas Conservation Commission. Production files by county and year: <http://wogcc.state.wy.us/productioncountyyear.cfm?Oops=#oops#&RequestTimeOut=6500>.

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## F.2. Overview of Treatment Processes for Treating Hydraulic Fracturing Wastewater

1 Treatment technologies discussed in this appendix are classified as basic or advanced. Basic  
2 treatment technologies are ineffective for reducing total dissolved solids (TDS) and are typically not  
3 labor intensive. Advanced treatment technologies can remove TDS and/or are complex in nature  
4 (e.g., energy- and labor-intensive).

### F.2.1. Basic Treatment

5 Basic treatment technologies include physical separation, coagulation/oxidation,  
6 electrocoagulation, sedimentation, and disinfection. These technologies are effective at removing  
7 total suspended solids (TSS), oil and grease, scale-forming compounds, and metals, and they can  
8 minimize microbial activity. Basic treatment is typically incorporated in a permanent treatment  
9 facility (i.e., fixed location) but can also be part of a mobile unit for onsite treatment applications.

#### F.2.1.1. Physical Separation

10 The most basic treatment need for oil and gas wastewaters, including those from hydraulic  
11 fracturing operations, is separation to remove suspended solids, and oil and grease. The separation  
12 method largely depends on the type of resource(s) targeted by the hydraulic fracturing operation.  
13 Down-hole separation techniques, including mechanical blocking devices and water shut-off  
14 chemicals to prevent or minimize water flow to the well, may be used during production in shale  
15 plays containing greater amounts of liquid hydrocarbons. To treat water at the surface, separation  
16 technologies such as hydrocyclones, dissolved air or induced gas flotation systems, media (sand)  
17 filtration, and biological aerated filters can remove suspended solids and some organics from  
18 hydraulic fracturing wastewater.

19 Media filtration can also remove hardness and some metals if chemical precipitation (i.e.,  
20 coagulation, lime softening) is also employed ([Boschee, 2014](#)). An example of a centralized waste  
21 treatment facility (CWT) that uses chemical precipitation and media filtration to treat hydraulic  
22 fracturing waste is the Water Tower Square Gas Well Wastewater Processing Facility in  
23 Pennsylvania (see Table 8-7). One or more of these technologies is typically used prior to advanced  
24 treatment such as reverse osmosis (RO) because advanced treatment processes foul, scale, or  
25 otherwise do not operate effectively in the presence of TSS, certain organics, and/or some metals  
26 and metalloid compounds ([Boschee, 2014](#); [Drewes et al., 2009](#)). The biggest challenge associated  
27 with use of these separation technologies is solids disposal from the resulting sludge ([Igunnu and](#)  
28 [Chen, 2014](#)).

#### F.2.1.2. Coagulation/Oxidation

29 Coagulation is the process of agglomerating small, un-settleable particles into larger particles to  
30 promote settling. Chemical coagulants such as alum, iron chloride, and polymers can be used to  
31 precipitate TSS, some dissolved solids (except monovalent ions such as sodium and chloride), and  
32 metals from hydraulic fracturing wastewater. Adjusting the pH using chemicals such as lime or  
33 caustic soda can increase the potential for some constituents, including dissolved metals, to form  
34 precipitates. Chemical precipitation is often used in industrial wastewater treatment as a

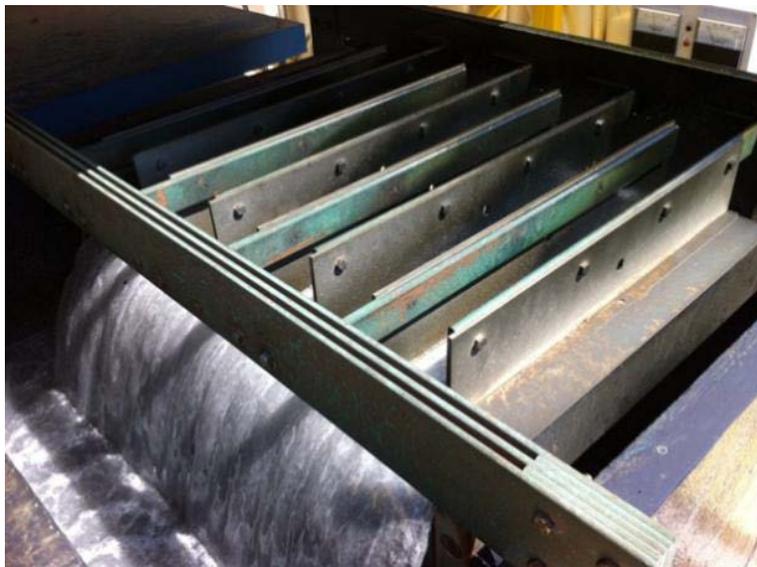
1 pretreatment step to decrease the pollutant loading on subsequent advanced treatment  
2 technologies; this strategy can save time, money, energy consumption and the lifetime of the  
3 infrastructure.

4 Processes using advanced oxidation and precipitation have been applied to hydraulic fracturing  
5 wastewaters in on-site and mobile systems. Hydroxyl radicals generated by cavitation processes  
6 and the addition of ozone can degrade organic compounds and inactivate micro-organisms. The  
7 process can also aid in the precipitation of elements, which cause hardness and scaling in the  
8 treated water (e.g. calcium, magnesium). The process can also reduce sulfate and carbonate  
9 concentrations in the treated water. This type of treatment can be very effective for on-site reuse of  
10 wastewater ([Ely et al., 2011](#)).

11 The produced solid residuals from coagulation/oxidation processes typically require further  
12 treatment, such as de-watering ([Duraisamy et al., 2013](#); [Hammer and VanBriesen, 2012](#)).

### **F.2.1.3. Electrocoagulation**

13 Electrocoagulation (EC) (Figure F-1) combines the principles of coagulation and electrochemistry  
14 into one process ([Gomes et al., 2009](#)). An electrical current added to the wastewater produces  
15 coagulants that then neutralize the charged particles, causing them to destabilize, precipitate, and  
16 settle. EC may be used in place of, or in addition to, chemical coagulation. EC can be effective for  
17 removal of organics, TSS, and metals, but it is less effective for removing TDS and sulfate. Although  
18 it is still considered an emerging technology for unconventional oil and gas wastewater treatment,  
19 EC has been used in mobile treatment systems to treat hydraulic fracturing wastewaters  
20 ([Halliburton, 2014](#); [Igunnu and Chen, 2014](#)). Limitations with this technology are the potential for  
21 scaling, corrosion, and bacterial growth ([Gomes et al., 2009](#)).



**Figure F-1. Electrocoagulation unit.**

Source: [Dunkel \(2013\)](#).

#### **F.2.1.4. Sedimentation**

1 Treatment plants may include sedimentation tanks, clarifiers, or some other form of settling basin  
2 to allow larger particles to settle out of the water where they can eventually be collected,  
3 dewatered, and disposed of. These types of tanks/basins all serve the same purpose – to reduce the  
4 amount of solids going to subsequent processes (i.e., overload the media filters).

#### **F.2.1.5. Disinfection**

5 Some hydraulic fracturing applications may require disinfection to kill bacteria after treatment and  
6 prior to reuse. Chlorine is a common disinfectant. Chlorine dioxide, ozone, or ultraviolet light can  
7 also be used. This is an important step for reused water because bacteria can cause problems for  
8 further hydraulic fracturing operations by multiplying rapidly and causing build-up in the well  
9 bore, which decreases gas extraction efficiency.

### **F.2.2. Advanced Treatment**

10 Advanced treatment technologies consist of membranes (reverse osmosis (RO), nanofiltration,  
11 ultrafiltration, microfiltration, electrodialysis, forward osmosis, and membrane distillation),  
12 thermal distillation technologies, crystallizers, ion exchange, and adsorption. These technologies  
13 are effective for removing TDS and/or targeted compounds. They typically require pretreatment to  
14 remove solids and other constituents that may damage or otherwise impede the technology from  
15 operating as designed. Advanced treatment technologies can be energy intensive and are typically  
16 employed when a purified water effluent is necessary for direct discharge, indirect discharge, or  
17 reuse. In some instances, these water treatment technologies can make use of methane generated  
18 by the gas well as an energy source. Some advanced treatment technologies can be made mobile for  
19 on-site treatment.

#### **F.2.2.1. Membranes**

20 Pressure-driven membrane processes including microfiltration, ultrafiltration, nanofiltration, and  
21 RO (Figure F-2) are being used in some settings to treat oil and gas wastewater. These processes  
22 use hydraulic pressure to overcome the osmotic pressure of the influent waste stream, forcing clean  
23 water through the membrane ([Drewes et al., 2009](#)). Microfiltration and ultrafiltration processes do  
24 not reduce TDS but can remove TSS and some metals and organics ([Drewes et al., 2009](#)). RO and  
25 nanofiltration are capable of removing TDS, including anions and radionuclides. RO, however, may  
26 be limited to treating TDS levels of approximately 40,000 mg/L TDS ([Shaffer et al., 2013](#); [Younos  
27 and Tulou, 2005](#)).



**Figure F-2. Photograph of reverse osmosis system.**

Source: Thinkstock.

#### ***F.2.2.2. Electrodialysis***

- 1 Electrodesialysis relies on positively and negatively charged particles and coated membranes to
- 2 separate contaminants from the water (Figure F-3). Electrodesialysis has been considered for use by
- 3 the shale gas industry, but it is not currently widely utilized ([ALL Consulting, 2013](#)). TDS
- 4 concentrations above 15,000 mg/L are difficult to treat by electrodesialysis ([ALL Consulting, 2013](#)),
- 5 and oil and divalent cations (e.g. Ca, Fe, Mg) can foul the membranes ([Hayes and Severin, 2012b](#);
- 6 [Guolin et al., 2008](#)).



**Figure F-3. Picture of mobile electro dialysis units in Wyoming.**

Source: [DOE \(2006\)](#). Permission: ALL Consulting.

#### **F.2.2.3. Forward Osmosis/Membrane Distillation**

1 Forward osmosis, an emerging technology for treating hydraulic fracturing wastewater, uses an  
2 osmotic pressure gradient across a membrane to draw the contaminants from a low osmotic  
3 solution (the feed water) to a high osmotic solution ([Drewes et al., 2009](#)). The selection of the  
4 constituents for the draw solution is very important as the constituents should be more easily  
5 removed from solution than the compounds (e.g. salts) in the feed. Alternatively, draw solutions can  
6 contain components that are more easily reused or recycled. Another emerging technology,  
7 membrane distillation, relies on a thermal gradient across a membrane surface to volatilize pure  
8 water and capture it in the distillate ([Drewes et al., 2009](#)).

#### **F.2.2.4. Thermal Distillation**

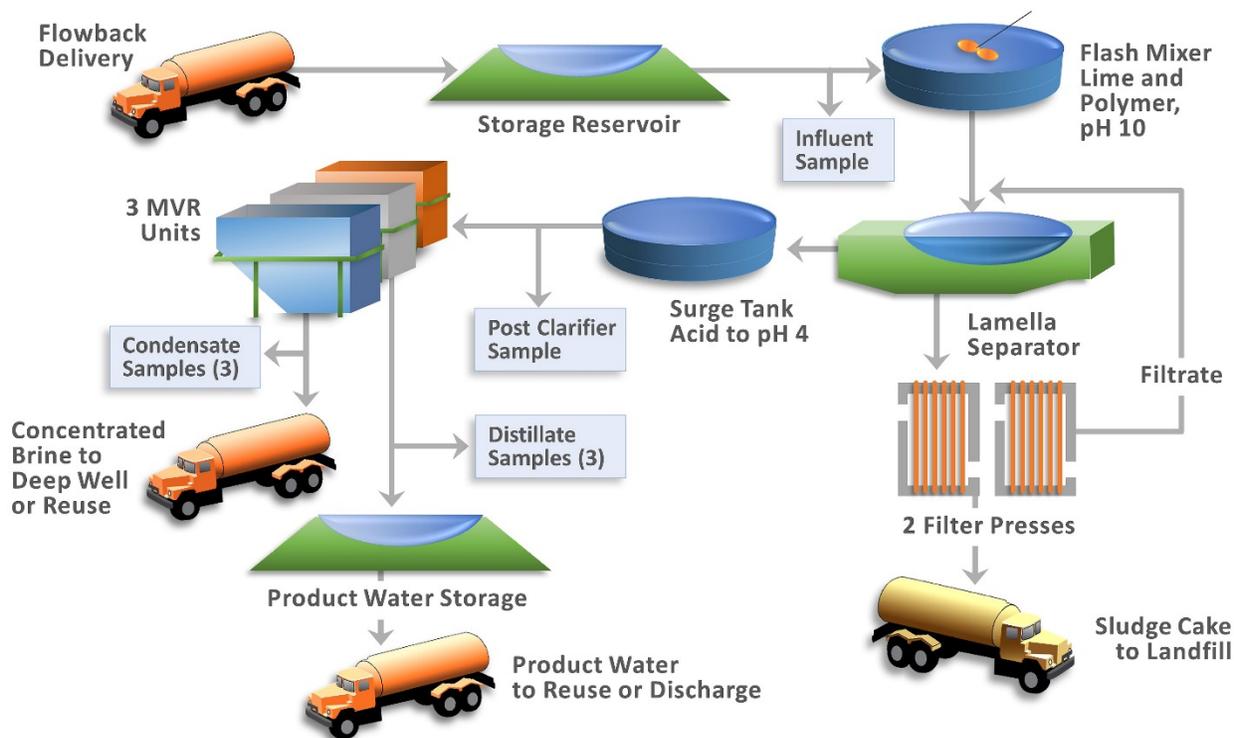
9 Thermal distillation technologies, such as mechanical vapor recompression (MVR) (Figure F-4) and  
10 dewvaporation, use liquid-vapor separation by applying heat to the waste stream, vaporizing the  
11 water to separate out impurities, and condensing the vapor into distilled water ([Drewes et al.,](#)  
12 [2009](#); [LEau LLC, 2008](#); [Hamieh and Beckman, 2006](#)). MVR and dewvaporation can treat high-TDS  
13 waters and have been proven in the field as effective for treating oil and gas wastewater ([Hayes and](#)  
14 [Severin, 2012b](#); [Drewes et al., 2009](#)). Like RO, these processes are energy intensive and are used  
15 when the objective is very clean water (i.e., TDS less than 500 mg/L) for direct/indirect discharge  
16 or if clean water is needed for reuse. As with membrane processes, scaling is an issue with these  
17 technologies, and scale inhibitors may be needed for them to operate effectively ([Igunnu and Chen,](#)  
18 [2014](#)).



**Figure F-4. Picture of a mechanical vapor recompression unit near Decatur, Texas.**

Source: [Drewes et al. \(2009\)](#). Permission provided.

- 1 CWTs such as the Judsonia Central Water Treatment Facility in Arkansas, and the Casella-Altela
- 2 Regional Environmental Services and Clarion Altela Environmental Services, both in Pennsylvania,
- 3 have NPDES permits and use MVR or thermal distillation for TDS removal. Figure F-5 shows a
- 4 diagram of the treatment train at another facility, the Maggie Spain facility in Texas, which uses
- 5 MVR in its treatment of Barnett Shale wastewater ([Hayes and Severin, 2012a](#)).



**Figure F-5. Mechanical vapor recompression process design – Maggie Spain Facility.**

Adapted from: [Hayes and Severin \(2012a\)](#).

- 1 Crystallizers can be employed at CWTs to treat high-TDS waters or to further concentrate the waste
- 2 stream from a distillation process, reducing residual waste disposal volumes. The crystallized salt
- 3 can be landfilled, deep-well injected, or used to produce pure salt products that may be salable
- 4 ([Ertel et al., 2013](#)).
- 5 Another thermal method, freeze-thaw evaporation, involves spraying wastewater onto a freezing
- 6 pad, allowing ice crystals to form, and the brine mixture that remains in solution to drain from the
- 7 ice ([Drewes et al., 2009](#)). In warmer weather, the ice thaws and the purified water is collected. This
- 8 technology cannot treat waters with high methanol concentrations and is only suitable for areas
- 9 where the temperature is below freezing in the winter months ([Igunnu and Chen, 2014](#)). In
- 10 addition, freeze-thaw evaporation can only reduce TDS concentrations to approximately 1,000
- 11 mg/L, which is higher than the 500 mg/L TDS surface water discharge limit required by most
- 12 permits ([Igunnu and Chen, 2014](#)).

#### **F.2.2.5. Ion Exchange and Adsorption**

- 13 Ion exchange (Figure F-6) is the process of exchanging ions on a media referred to as resin for
- 14 unwanted ions in the water. Ion exchange is used to treat for target ions that may be difficult to
- 15 remove by other treatment technologies or that may interfere with the effectiveness of advanced
- 16 treatment processes.



**Figure F-6. Picture of a compressed bed ion exchange unit.**

Source: [Drewes et al. \(2009\)](#). Permission provided.

- 1 Adsorption is the process of adsorbing contaminants onto a charged granular media surface.
- 2 Adsorption technologies can effectively remove organics, heavy metals, and some anions ([Igunnu](#)
- 3 [and Chen, 2014](#)). With ion exchange and adsorption processes, the type of resin or adsorptive
- 4 media used (e.g., activated carbon, organoclay, zeolites) dictates the specific contaminants that will
- 5 be removed from the water ([Drewes et al., 2009](#); [Fakhru'l-Razi et al., 2009](#)).
  
- 6 Because they can be easily overloaded by contaminants, ion exchange and adsorption treatment
- 7 processes are generally used as a polishing step following other treatment processes or as a unit
- 8 process in a treatment train rather than as stand-alone treatment ([Drewes et al., 2009](#)). Stand-alone
- 9 units require more frequent regeneration and/or replacement of the spent media making these
- 10 technologies more costly to operate ([Igunnu and Chen, 2014](#)). Figure F-7 shows a schematic of the
- 11 Pinedale Anticline Water Reclamation Facility located in Wyoming, which uses an ion exchange unit
- 12 with boron-selective resin as a polishing step to treat hydraulic fracturing wastewater specifically
- 13 for boron ([Boschee, 2012](#)).

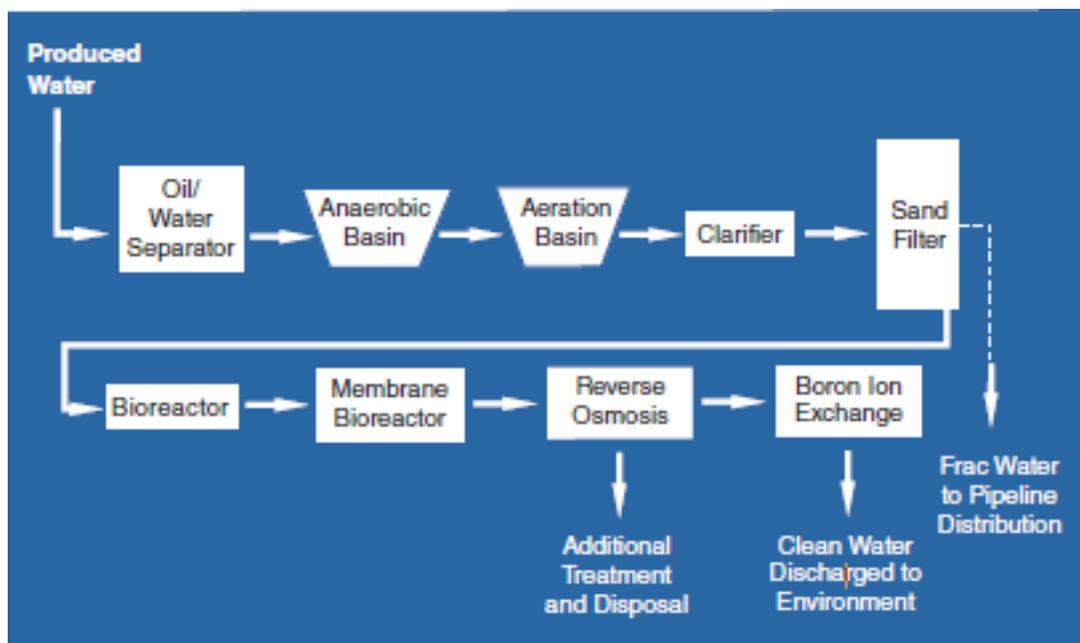


Figure F-7. Discharge water process used in the Pinedale Anticline field.

Source: [Boschee \(2012\)](#).

### F.3. Treatment Technology Removal Capabilities

1 Table F-2 provides removal efficiencies for common hydraulic fracturing wastewater constituents  
 2 by treatment technology. With the exception of TSS and TDS, the studies cited demonstrate removal  
 3 for a subset of constituents in a category (e.g., [Gomes et al., 2009](#)) reported that electro dialysis was  
 4 an effective treatment for oil and grease, not all organics). The removal efficiencies include ranges  
 5 of 1 to 33% (denoted by +), 34% to 66% (denoted by ++), and greater than 66% removal (denoted  
 6 by +++). Cells denoted with "--" indicate that the treatment technology is not suitable for removal of  
 7 that constituent or group of constituents. If a particular treatment technology only lists removal  
 8 efficiencies for TDS, it can be assumed that in some cases, cations and anions would also be  
 9 removed by that technology; therefore, where specific results were not provided in literature, cells  
 10 denoted with "Assumed" refer to cations and anions that comprise TDS.

**Table F-2. Removal efficiency of different hydraulic fracturing wastewater constituents using various wastewater treatment technologies.<sup>a</sup>**

Treatment Technology	Hydraulic Fracturing Wastewater Constituents					
	TSS	TDS	Anions	Metals	Radio-nuclides	Organics
Hydrocyclones	+++ ( <a href="#">Duraisamy et al., 2013</a> )	--	--	--	--	++ ( <a href="#">Duraisamy et al., 2013</a> )
Evaporation (freeze-thaw evaporation)	+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Drewes et al., 2009</a> )	+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Drewes et al., 2009</a> ; <a href="#">Arthur et al., 2005</a> )	Assumed	+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Drewes et al., 2009</a> ; <a href="#">Arthur et al., 2005</a> )	--	+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Duraisamy et al., 2013</a> ; <a href="#">Drewes et al., 2009</a> )
Filtration (granular media)	+++ ( <a href="#">Barrett, 2010</a> )	--	--	+++ <sup>b</sup> ( <a href="#">Duraisamy et al., 2013</a> )	--	+++ ( <a href="#">Shafer, 2011</a> ; <a href="#">Drewes et al., 2009</a> )
Chemical precipitation	+++ ( <a href="#">Fakhru'l-Razi et al., 2009</a> )	--	--	+++ ( <a href="#">Fakhru'l-Razi et al., 2009</a> ; <a href="#">AWWA, 1999</a> )	+++ <sup>c</sup> ( <a href="#">Zhang et al., 2014</a> )	+++ ( <a href="#">Fakhru'l-Razi et al., 2009</a> )
Sedimentation (clarifier)	++ ( <a href="#">NMSU DACC WUTAP, 2007</a> )	--	--	--	--	--
Dissolved air flotation	+++ ( <a href="#">Shammas, 2010</a> )	--	--	--	--	++/+++ ( <a href="#">Duraisamy et al., 2013</a> ; <a href="#">Fakhru'l-Razi et al., 2009</a> )
Electro-coagulation	+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Bukhari, 2008</a> )	--	--	+ ( <a href="#">Igunnu and Chen, 2014</a> )	--	+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Duraisamy et al., 2013</a> ; <a href="#">Fakhru'l-Razi et al., 2009</a> )
Advanced oxidation and precipitation	--	+ ( <a href="#">Abrams, 2013</a> )	--	+ /+++ ( <a href="#">Abrams, 2013</a> )	--	+++ <sup>d</sup> ( <a href="#">Duraisamy et al., 2013</a> ) ( <a href="#">Fakhru'l-Razi et al., 2009</a> )

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Treatment Technology	Hydraulic Fracturing Wastewater Constituents					
	TSS	TDS	Anions	Metals	Radio-nuclides	Organics
Reverse osmosis	--	++/+++ <sup>e</sup> ( <a href="#">Alzahrani et al., 2013</a> ; <a href="#">Drewes et al., 2009</a> )	+++ ( <a href="#">Alzahrani et al., 2013</a> ) ( <a href="#">Arthur et al., 2005</a> )	++/+++ <sup>f</sup> ( <a href="#">Alzahrani et al., 2013</a> ) ( <a href="#">Drewes et al., 2009</a> ; <a href="#">AWWA, 1999</a> )	+++ ( <a href="#">Drewes et al., 2009</a> )	+//+/+++ <sup>g</sup> ( <a href="#">Drewes et al., 2009</a> ; <a href="#">Munter, 2000</a> )
Membrane filtration (UF/MF)	+++ ( <a href="#">Arthur et al., 2005</a> )	--	--	+++ ( <a href="#">Fakhru'l-Razi et al., 2009</a> )	--	++/+++ ( <a href="#">Duraismy et al., 2013</a> ; <a href="#">Fakhru'l-Razi et al., 2009</a> ; <a href="#">Hayes and Arthur, 2004</a> ; <a href="#">AWWA, 1999</a> ) <sup>h</sup>
Forward osmosis	--	+++ ( <a href="#">Drewes et al., 2009</a> )	Assumed	Assumed	--	--
Distillation, including thermal distillation (e.g., mechanical vapor recompression (MVR))		+++ <sup>i</sup> ( <a href="#">Hayes et al., 2014</a> ; <a href="#">Bruff and Jikich, 2011</a> ; <a href="#">Drewes et al., 2009</a> )	+++ ( <a href="#">Bruff and Jikich, 2011</a> ; <a href="#">Drewes et al., 2009</a> )	+++ ( <a href="#">Hayes et al., 2014</a> ; <a href="#">Bruff and Jikich, 2011</a> ; <a href="#">Drewes et al., 2009</a> )	+++ ( <a href="#">Bruff and Jikich, 2011</a> ; <a href="#">Drewes et al., 2009</a> )	+//+/+++ ( <a href="#">Hayes et al., 2014</a> ; <a href="#">Duraismy et al., 2013</a> ; <a href="#">Drewes et al., 2009</a> ; <a href="#">Fakhru'l-Razi et al., 2009</a> )
Ion exchange	--	--	+++ ( <a href="#">Drewes et al., 2009</a> )	+++ ( <a href="#">Drewes et al., 2009</a> ; <a href="#">Arthur et al., 2005</a> )	+++ ( <a href="#">Drewes et al., 2009</a> )	+//+/+++ ( <a href="#">Fakhru'l-Razi et al., 2009</a> ; <a href="#">Munter, 2000</a> ) <sup>j</sup>
Crystallization	--	+++ ( <a href="#">ER, 2014</a> )	Assumed	Assumed	--	--
Electrodialysis	--	+++ <sup>k</sup> ( <a href="#">Drewes et al., 2009</a> ; <a href="#">Gomes et al., 2009</a> ; <a href="#">Arthur et al., 2005</a> )	++/+++ ( <a href="#">Banasiak and Schäfer, 2009</a> )	+//+/+++ ( <a href="#">Banasiak and Schäfer, 2009</a> )	--	+++ ( <a href="#">Gomes et al., 2009</a> )
Capacitive deionization (emerging technology)	--	+++ <sup>l</sup> ( <a href="#">Drewes et al., 2009</a> )	--	--	--	--

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Treatment Technology	Hydraulic Fracturing Wastewater Constituents					
	TSS	TDS	Anions	Metals	Radio-nuclides	Organics
Adsorption <sup>m</sup>	--	--	+ /++ /+++ <sup>n</sup> ( <a href="#">Habuda-Stanic et al., 2014</a> )	+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Drewes et al., 2009</a> )	--	+ /++ /+++ ( <a href="#">Arthur et al., 2005</a> ; <a href="#">Hayes and Arthur, 2004</a> ; <a href="#">Munter, 2000</a> )
Biological treatment	+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Drewes et al., 2009</a> )	--	--	--	--	+ /++ /+++ ( <a href="#">Igunnu and Chen, 2014</a> ; <a href="#">Drewes et al., 2009</a> ; <a href="#">Fakhru'l-Razi et al., 2009</a> )
Constructed wetland/reed beds	++ /+++ ( <a href="#">Manios et al., 2003</a> )	+ ( <a href="#">Arthur et al., 2005</a> )	--	++ /+++ ( <a href="#">Fakhru'l-Razi et al., 2009</a> )	--	+ /+++ ( <a href="#">Fakhru'l-Razi et al., 2009</a> ; <a href="#">Arthur et al., 2005</a> )

<sup>a</sup> To the extent possible, removal efficiencies are based on an individual treatment technology that does not assume extensive pretreatment or combined treatment processes. However, it should be noted that some processes cannot effectively operate without pretreatment (e.g., RO, media filtration, sedimentation).

<sup>b</sup> Pretreatment (pH adjustment, aeration, solids separation) required.

<sup>c</sup> Radium co-precipitation with barium sulfate.

<sup>d</sup> The Fenton process.

<sup>e</sup> Typically requires pretreatment. Not a viable technology if TDS influent >50,000 mg/L.

<sup>f</sup> Iron and manganese oxides will foul the membranes.

<sup>g</sup> Some organics will foul the membranes (e.g., organic acids).

<sup>h</sup> Ultrafiltration membrane was modified with nanoparticles.

<sup>i</sup> Can typically handle high TDS concentrations.

<sup>j</sup> Resin consisted of modified zeolites that targeted removal of BTEX.

<sup>k</sup> Influent TDS for this technology should be <8,000 mg/L.

<sup>l</sup> Specific technology was an electronic water purifier which is a hybrid of capacitive deionization. Influent TDS for this technology should be <3,000 mg/L.

<sup>m</sup> Typically polishing step, otherwise can overload bed quickly with organics.

<sup>n</sup> Removal efficiency is dependent on the type of adsorbent used and the water quality characteristics (e.g., pH).

- 1 Given the variety of properties among classes of organic constituents, different treatment processes
- 2 may be required depending upon the types of organic compounds needing removal. Table F-3 lists
- 3 treatment processes and the classes of organic compounds they can treat.

**Table F-3. Treatment processes for hydraulic fracturing wastewater organic constituents.**

Treatment processes	Organic compounds removed	References
Adsorption with activated carbon	Soluble organic compounds	<a href="#">Fakhru'l-Razi et al. (2009)</a>
Adsorption with organoclay media	Insoluble organic compounds	<a href="#">Fakhru'l-Razi et al. (2009)</a>
Aeration	Volatile organic compounds	<a href="#">Tchobanoglous et al. (2013)</a>
Dissolved air flotation	Volatile organic compounds, dispersed oil	<a href="#">Drewes et al. (2009)</a>
Freeze/thaw evaporation <sup>a</sup>	TPH, volatile organic compounds, semi-volatile organic compounds	<a href="#">Duraismy et al. (2013)</a> ; <a href="#">Drewes et al. (2009)</a>
Ion exchange (with modified zeolites)	BTEX, chemical oxygen demand, biochemical oxygen demand	<a href="#">Hayes et al. (2014)</a> ; <a href="#">Duraismy et al. (2013)</a> ; <a href="#">Drewes et al. (2009)</a> ; <a href="#">Fakhru'l-Razi et al. (2009)</a> ; <a href="#">Munter (2000)</a>
Distillation	BTEX, polycyclic aromatic hydrocarbons (PAHs)	<a href="#">Hayes et al. (2014)</a> ; <a href="#">Duraismy et al. (2013)</a> ; <a href="#">Drewes et al. (2009)</a> ; <a href="#">Fakhru'l-Razi et al. (2009)</a> .
Chemical precipitation	Oil & grease	<a href="#">Drewes et al. (2009)</a> ; <a href="#">Fakhru'l-Razi et al. (2009)</a>
Chemical Oxidation	Oil & grease	<a href="#">Drewes et al. (2009)</a> ; <a href="#">Fakhru'l-Razi et al. (2009)</a>
Media filtration (walnut shell media or sand)	Oil & grease	<a href="#">Drewes et al. (2009)</a> ; <a href="#">Fakhru'l-Razi et al. (2009)</a>
Microfiltration	Oil & grease	<a href="#">Drewes et al. (2009)</a> ; <a href="#">Fakhru'l-Razi et al. (2009)</a>
Ultrafiltration	Oil & grease, BTEX	<a href="#">Drewes et al. (2009)</a> ; <a href="#">Fakhru'l-Razi et al. (2009)</a>
Reverse osmosis <sup>b</sup>	Dissolved organics	<a href="#">Drewes et al. (2009)</a> ; <a href="#">U.S. EPA (2005)</a>
Electrocoagulation	Chemical oxygen demand, Biochemical oxygen demand	<a href="#">Fakhru'l-Razi et al. (2009)</a>
Biologically aerated filters	Oil & grease, TPH, BTEX	<a href="#">Fakhru'l-Razi et al. (2009)</a>
Reed bed technologies	Oil & grease, TPH, BTEX	<a href="#">Fakhru'l-Razi et al. (2009)</a>
Hydrocyclone separators	Dispersed oil	<a href="#">Drewes et al. (2009)</a>

<sup>a</sup> Technology cannot be used if the methanol concentration in the hydraulic fracturing wastewater exceeds 5%.

<sup>b</sup> RO will remove specific classes of organic compounds with removal efficiencies dependent on the compound's structure and the physical and chemical properties of the hydraulically fractured wastewater. Organoacids will foul membranes.

- 1 Table F-4 presents estimated effluent concentrations that could be produced by a variety of unit
- 2 treatment processes for several example constituents and for various influent concentrations. This

1 analysis uses treatment process removal efficiencies from literature used to develop Table F-2 and  
2 average wastewater concentrations of several constituents presented in Chapter 7 and Appendix E.  
3 These estimates were done to illustrate the combined effects of influent wastewater composition  
4 and treatment process choice on achievable effluent concentrations. The removal efficiencies  
5 represent a variety of studies, primarily at bench and pilot scale, and done with either conventional  
6 or hydraulic fracturing wastewater. Removal efficiency for a given treatment process can vary due  
7 to a number of factors, and constituent removal may be different in a full-scale facility that uses  
8 several processes. Thus, the calculations shown in Table F-4 are intended to be rough  
9 approximations for illustrative purposes.



Shale/ Sandstone Play	Contaminant	MCL	Avg. Influent Conc.	Units	Freeze-Thaw Evaporation	Media Filtration	Chemical Precipitation	Flotation (DAF)	Electro-coagulation	Advanced Oxidation and precipitation	Reverse osmosis	Membrane Filtration (UF/MF)	Distillation	Ion exchange	Electrodialysis	Adsorption	Biological Treatment (bioreactors, BAFs)	Constructed Wetland
Devonian Sandstone	Radium 226	--	2400	pCi/L			120 - 1700				24		24 - 71	170				
Marcellus	Radium 228	--	120	pCi/L			6.2 - 85				1.2		1.2 - 3.6	8.4				
Marcellus	Total Radium	<b>5</b>	2500	pCi/L			130 - 1800				25		25 - 76	180				
Barnett	TOC	--	9.8	mg/L								0.2				0.98 - 2.9	2.1 - 4	1
Marcellus	TOC	--	160	mg/L								3.2				16 - 48	35 - 58	16
Cotton Valley	TOC	--	200	mg/L								4				20 - 59	44 - 71	20
Barnett	BOD	--	580	mg/L					58					290 - 440			29 - 87	47
Marcellus	BOD	--	40	mg/L					4					20 - 30			2 - 6	3.2
Barnett	O&G	--	160	mg/L		16						16			8	1.6	43	9.8
Marcellus	O&G	--	74	mg/L		7.4						7.4			3.7	0.74	19	4.4
Barnett	Benzene	<b>5</b>	680	µg/L	68							310	6.8			110		ND
Marcellus	Benzene	<b>5</b>	360	µg/L	36							170	3.6			58		ND
Barnett	Toluene	<b>1,000</b>	760	µg/L	76							350				84		ND
Marcellus	Toluene	<b>1,000</b>	1100	µg/L	110							510				120		ND
Barnett	Ethylbenzene	<b>700</b>	29	µg/L	2.9											3.2		ND
Marcellus	Ethylbenzene	<b>700</b>	150	µg/L	15											17		ND
Barnett	Xylenes	<b>10,000</b>	360	µg/L	36							170				14		ND
Marcellus	Xylenes	<b>10,000</b>	1300	µg/L	130							600				52		ND
Barnett	BTEX	--	1800	µg/L	180				7.3				91	270 - 550	3.7 - 91			

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Shale/ Sandstone Play	Contaminant	MCL	Avg. Influent Conc.	Units	Freeze-Thaw Evaporation	Media Filtration	Chemical Precipitation	Flotation (DAF)	Electro-coagulation	Advanced Oxidation and precipitation	Reverse osmosis	Membrane Filtration (UF/MF)	Distillation	Ion exchange	Electrolysis	Adsorption	Biological Treatment (bioreactors, BAFs)	Constructed Wetland
Marcellus	BTEX	--	2900	µg/L	290					12			150	440 - 870		5.8 - 150		
Barnett	Naphthalene	--	240	µg/L						0.95								
Marcellus	Naphthalene	--	360	µg/L						1.4								
Barnett	1,2,4-Trimethylbenzene	--	170	µg/L						0.69								
Marcellus	1,2,4-Trimethylbenzene	--	430	µg/L						1.7								
Barnett	1,2,4-Trimethylbenzene	--	59	µg/L						0.24								
Marcellus	1,2,4-Trimethylbenzene	--	310	µg/L						1.2								

ND = Non-detect

#### F.4. Centralized Waste Treatment Facilities and Waste Management Options

1 CWTs are designed to treat for site-specific wastewater constituents so that the effluent meets the  
2 requirements of the designated disposal option(s) (i.e., reuse, direct/indirect discharge). The most  
3 basic treatment processes that a CWT might use include ([Easton, 2014](#); [Duhon, 2012](#)):

- 4 • Physical treatment technologies such as dissolved air or gas flotation technologies, media  
5 filtration, hydrocyclones, and clarification;
- 6 • Chemical treatment technologies such as chemical precipitation and chemical oxidation;  
7 and
- 8 • Biological treatment technologies such as biological aerated filter systems and reed beds.

9 While these technologies are effective at removing oil and grease, suspended solids, scale-forming  
10 compounds, and some heavy metals, if TDS should be reduced as required by the intended disposal  
11 option, advanced processes such as RO, thermal distillation, or evaporation are necessary.

##### F.4.1. Discharge Options for CWTs

12 Direct discharge CWTs are allowed to discharge treated wastewater directly to surface waters  
13 under the NPDES permit program. Discharge limitations may be based on water quality standards  
14 in the NPDES and technology-based effluent limitation guidelines under 40 CFR Part 437. In  
15 addition, permitting authorities have permitted facilities for discharge under 40 CFR 435, Subpart  
16 E. Judsonia Central Water Treatment Facility in Sunnydale, Arkansas is permitted to directly  
17 discharge treated effluent from produced and flowback waters from the Fayetteville Shale play to  
18 Byrd pond located on the property. Pinedale Anticline Field Wastewater Treatment Facility in  
19 Wyoming, WY, originally designed to treat produced water from tight gas plays in the Pinedale  
20 Anticline Field to levels suitable for reuse, was upgraded to include RO treatment for discharge to a  
21 local river. CWTs with NPDES discharge permits may also opt to treat oil and gas wastewater for  
22 reuse. Some facilities have the ability to treat wastewater to different qualities (e.g., with or without  
23 TDS removal), which they might do to target various reuse water quality criteria. Both the Judsonia  
24 facility and Pinedale facility discussed above have the ability to employ either TDS- or non-TDS-  
25 removal treatment depending on the customers' needs.

26 Indirect discharge CWTs may treat hydraulic fracturing wastewater and then discharge the treated  
27 wastewater effluent to a POTW. Discharge to the POTW is controlled by an Industrial User  
28 mechanism, which incorporates pretreatment standards established in 40 CFR Part 437. Two  
29 facilities located in Pennsylvania (Eureka Resources) and Ohio (Patriot Water Treatment) include  
30 indirect discharge as an option in wastewater treatment. The Eureka-Williamsport facility accepts  
31 wastewater (primarily from the Marcellus Shale play) and either treats it for reuse or discharges it  
32 to the local POTW. The Patriot facility offers services to hydraulic fracturing operators in the  
33 Marcellus and Utica Shale plays for removal of solids and metals using chemical treatment. As of  
34 March 2015, however, the Patriot facility is limited by the Ohio Environmental Protection Agency in  
35 accepting only "low salinity" (<50,000 mg/L TDS) produced water and may only discharge 100,000  
36 gallons (380,000 L) per day to the Warren Ohio POTW.

1 Zero-discharge CWTs do not discharge treated wastewater; instead, the wastewater is treated and  
 2 reused in subsequent hydraulic fracturing operations. [WVWRI \(2012\)](#) state that this practice  
 3 reduces potential effects on surface drinking water sources by reducing both direct and indirect  
 4 discharges. Zero-discharge facilities may offer different levels of treatment including minimal  
 5 treatment (for example, filtration), low-level treatment (chemical precipitation), and/or advanced  
 6 treatment (evaporation, crystallization). Reserved Environmental Services (RES) Mt. Pleasant,  
 7 Pennsylvania, is a zero liquid discharge facility permitted by PA DEP to treat wastewater from the  
 8 Marcellus Shale play for reuse. Residual solids are dewatered and sent to a landfill. Treated  
 9 wastewater effluent is stored, monitored, and chlorinated for reuse ([ONG Services, 2015](#)).

### F.5. Water Quality for Reuse

10 As of 2015, there is no consensus on the water quality requirements for reuse of wastewater for  
 11 hydraulic fracturing, and operator opinions vary on the minimum standards for the water quality  
 12 needed for fracturing fluids ([Vidic et al., 2013](#); [Acharya et al., 2011](#)). Table F-5 provides a list of  
 13 constituents and the recommended or observed target concentrations for reuse applications. The  
 14 wide concentration ranges for many constituents (e.g., TDS ranges from 500 to 70,000 mg/L),  
 15 suggest that water quality requirements for reuse are dictated by operation-specific requirements,  
 16 including operator preference and selection of fracturing fluid chemistry.

**Table F-5. Water quality requirements for reuse.**

Source: [U.S. EPA \(2015g\)](#).

Constituent	Reasons for Limiting Concentrations	Recommended or observed base fluid target concentrations (mg/L, after blending) <sup>b</sup>
TDS	Fluid stability	500 – 70,000
Chloride	Fluid stability	2,000 – 90,000
Sodium	Fluid stability	2,000 – 5,000
<i>Metals</i>		
Iron	Scaling	1 – 15
Strontium	Scaling	1
Barium	Scaling	2 – 38
Silica	Scaling	20
Calcium	Scaling	50 – 4,200
Magnesium	Scaling	10 – 1,000
Sulfate	Scaling	124 – 1,000
Potassium	Scaling	100 – 500
Scale formers <sup>a</sup>	Scaling	2,500

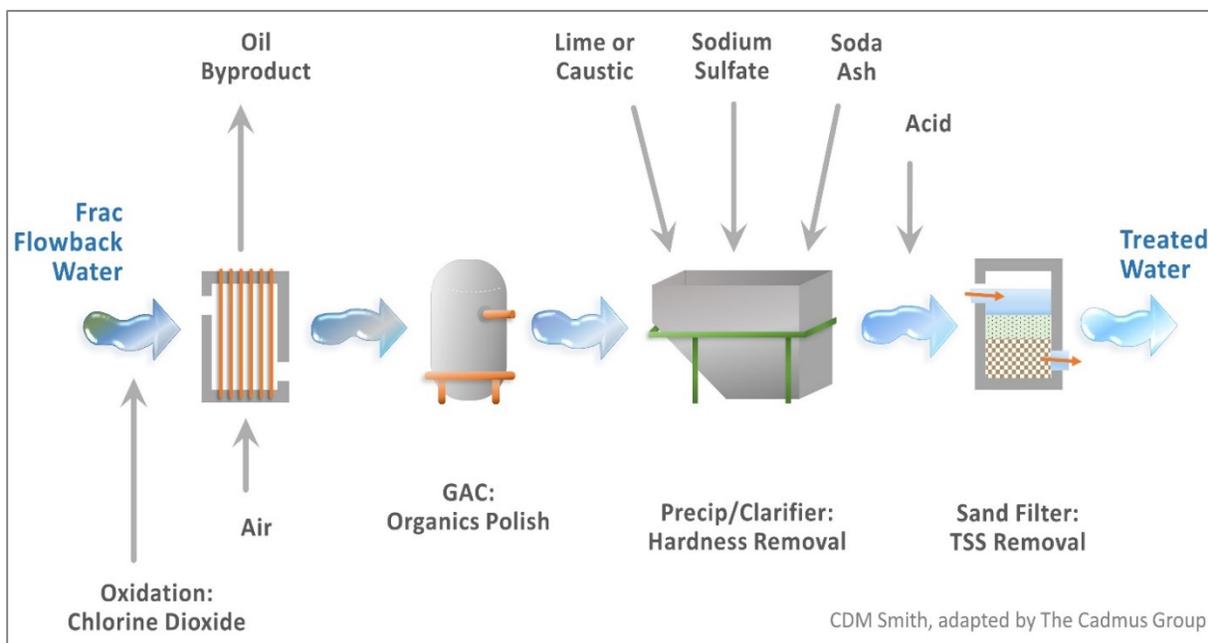
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Constituent	Reasons for Limiting Concentrations	Recommended or observed base fluid target concentrations (mg/L, after blending) <sup>b</sup>
<b>Other</b>		
Phosphate	Not Reported	10
TSS	Plugging	50 – 1,500
Oil	Fluid stability	5 – 25
Boron	Fluid stability	0 – 10
pH (S.U.)	Fluid stability	6.5 – 8.1
Bacteria (counts/mL)	Bacterial growth	0 – 10,000

<sup>a</sup> Includes total of barium, calcium, manganese, and strontium.

<sup>b</sup> Unless otherwise noted.

1 Wastewater quality can be managed for reuse by either blending it with freshwater and allowing  
2 dilution to bring the concentrations of problematic constituents to an acceptable range or through  
3 treatment ([Veil, 2010](#)). Treatment, if needed, can be conducted at facilities that are mobile, semi-  
4 permanent modular systems, or fully permanent CWTs ([Nicot et al., 2012](#)). At a minimum, hydraulic  
5 fracturing service providers generally prefer that the wastewater be treated to remove TSS,  
6 microorganisms, and constituents that form scale or inhibit crosslinking in gelled fluid systems  
7 ([Boschee, 2014](#)). Figure F-8 shows a schematic of a treatment system to treat wastewater for reuse  
8 that can remove suspended solids, hardness, and organic constituents.



**Figure F-8. Diagram of treatment for reuse of flowback and produced water.**

Source: [Kimball \(2010\)](#).

- 1 In the Marcellus, the wastewater to be reused is first generally treated with oil/gas-water  
 2 separation, filtration, and dilution ([Ma et al., 2014](#)). Although many Marcellus treatment facilities  
 3 only supply basic reuse treatment that removes oil and solids, advanced treatment facilities that  
 4 use techniques such as RO or distillation methods are also in operation ([Veil, 2010](#)).
- 5 Reuse concerns can vary with the type of hydraulic fracturing fluid used (e.g., slickwater, linear gel,  
 6 crosslinked gel, foam) ([Wasylishen and Fulton, 2012](#)) and the anticipated changes in water  
 7 chemistry over time (transition from flowback to produced water) ([Hammer and VanBriesen,  
 8 2012](#)). Elevated TDS is a concern, but residual constituents from previous fluid mixtures (e.g.,  
 9 breakers) may also cause difficulties when reusing water for subsequent fracturing operations  
 10 ([Montgomery, 2013](#); [Walsh, 2013](#)).
- 11 *On-Site Treatment for Reuse*
- 12 On-site systems that treat produced water for reuse can reduce potential impacts to drinking water  
 13 resources associated with transportation and disposal and facilitate the logistics of reuse by  
 14 preparing the water close to well sites. These systems sometimes consist of mobile units containing  
 15 one or more treatment processes that can be moved from site to site to treat waters in newly  
 16 developed sites that are not yet producing at full-scale. Semi-permanent facilities that serve a  
 17 specific area also exist ([Halldorson, 2013](#); [Boschee, 2012](#)).
- 18 Treatment systems are typically tailored for site-specific produced water chemical concentrations  
 19 and desired water quality treatment goals, including whether significant TDS removal is needed. If

1 low TDS water is needed, more advanced treatment will be required (see Section 8.5 of Chapter 8),  
2 which can increase the treatment costs to three to four times higher than for treatment systems  
3 that do not remove TDS ([Halldorson, 2013](#)). On-site facilities may be warranted where truck  
4 hauling or seasonal accessibility to and from a central facility is an issue ([Boschee, 2014](#); [Tiemann  
et al., 2014](#)). Operators may also consider on-site facilities if they have not fully committed to an  
5 area and the well counts are initially low. In those instances, they can later decide to add or remove  
6 units based on changing production volumes ([Boschee, 2014](#)).  
7

## F.6. Hydraulic Fracturing Impacts on POTWs

### F.6.1. Potential Impacts on Treatment Processes

8 Wastewater treatment processes used by POTWs are generally not designed or operated for  
9 wastewater containing high salt concentrations (>0.1-5% salt). Four basic problems for biological  
10 treatment of saline water have been described ([Woolard and Irvine, 1995](#)): 1) microbes in  
11 conventional treatment systems tend to be sensitive to changes in ionic strength, 2) microbial  
12 metabolic functions are disrupted leading to decreased degradation of carbon compounds, 3)  
13 effluent suspended solids are increased due to cell lysis and/or a reduction in organisms that  
14 promote flocculation, and 4) the extent of salt acclimation is limited in conventional systems.

15 Biological pre-treatment may be beneficial as an added process in pre-treatment (e.g. prior to  
16 indirect discharge from a CWT to a POTW) for removal of organic contaminants. Specialized  
17 treatment systems using salt-tolerant bacteria may be beneficial as an additional level of treatment  
18 for pre-treating (or polishing) wastewaters in centralized treatment systems. (These processes  
19 differ from conventional biological processes in standard wastewater treatment, which are not  
20 suitable for large volumes of UOG wastewater.) In particular, membrane bioreactors (MBRs) have  
21 been examined for the treatment of oil and gas wastewater ([Dao et al., 2013](#); [Kose et al., 2012](#);  
22 [Miller, 2011](#)). MBRs provide advantages over conventional aeration basin processes as they can be  
23 implemented into existing treatment trains more easily and have a much smaller footprint than  
24 aeration basins.

25 Because sudden increases in chloride concentration, above 5-8 g/L, may cause problems for  
26 wastewater treatment ([Ludzack and Noran, 1965](#)). POTWs planning to accept indirect discharge in  
27 the future may find it valuable to restrict influent salt concentrations to a level that will not disturb  
28 existing biological treatment processes.

## F.7. Hydraulic Fracturing and DBPs

### F.7.1.1. Disinfection By-Products

29 This section provides background information on disinfection by-products (DBPs) and their  
30 formation to support the discussion in Section 8.6.1 of Chapter 8 regarding impacts on surface  
31 waters and downstream drinking water utilities due to elevated bromide and iodide in hydraulic  
32 fracturing wastewaters.

1 Regulated DBPs are a small subset of the full spectrum of DBPs that include other chlorinated and  
2 brominated DBPs as well as nitrogenous and iodated DBPs. Some of the emerging unregulated  
3 DBPs may be more toxic than their regulated counterparts ([Harkness et al., 2015](#); [McGuire et al.,  
4 2014](#); [Parker et al., 2014](#)). Of the many types of DBPs that can form when drinking water is  
5 disinfected, SDWA's Stage 1 and Stage 2 DBP Rules regulate four total trihalomethanes (TTHMs),  
6 five haloacetic acids (HAA5s), bromate, and chlorite ([U.S. EPA, 2006](#)).

7 Most brominated DBPs form when water containing organic material and bromide reacts with a  
8 disinfectant such as chlorine during drinking water treatment. Parameters that affect DBP  
9 formation include concentration and type of organic material, disinfectant concentration, pH, water  
10 temperature, and disinfectant contact time. In addition, many studies have found that elevated  
11 bromide levels correlate with increased DBP formation ([Singer, 2010](#); [Obolensky and Singer, 2008](#);  
12 [Matamoros et al., 2007](#); [Hua et al., 2006](#); [Yang and Shang, 2004](#)). Some studies found similar results  
13 for iodide as well ([McGuire et al., 2014](#); [Parker et al., 2014](#)). [Pope et al. \(2007\)](#) reported that  
14 increased bromide levels are the second best indicator of DBP formation, with pH being the first.

15 In addition, research finds that higher levels of bromide and iodide contribute to increased  
16 concentrations of the brominated and iodated forms of DBPs (both regulated and unregulated),  
17 which tend to be more cytotoxic, genotoxic, and carcinogenic than chlorinated species ([McGuire et  
18 al., 2014](#); [Parker et al., 2014](#); [States et al., 2013](#); [Krasner, 2009](#); [Richardson et al., 2007](#)). Studies  
19 generally report that the ratios of halogen incorporation into DBPs reflect the ratio of halogen  
20 concentrations in the source water ([Criquet et al., 2012](#); [Jones et al., 2012](#); [Obolensky and Singer,  
21 2008](#)).

22 From a regulatory perspective, elevated bromide levels create difficulties in meeting drinking water  
23 MCLs. When the TTHMs are predominately in the form of brominated DBPs, the higher molecular  
24 weight of bromide (79.9 g/mol) relative to chloride (35.5 g/mol) causes the overall mass of the  
25 TTHM sum to increase. This can lead to elevated concentrations of TTHM, in turn potentially  
26 leading to violations of the TTHM MCL for the drinking water utility ([Francis et al., 2009](#)).

27 High bromide levels are also cited as causing formation of nitrogenous DBP N-  
28 nitrosodimethylamine (NDMA) in water disinfected with chloramines ([Luh and Mariñas, 2012](#)).  
29 Although NDMA is not regulated by the EPA as of early 2015, it is listed as a priority toxic pollutant,  
30 and the EPA is planning to evaluate NDMA and other nitrosamines as candidates for regulation  
31 during the six-year review of the Microbial and Disinfection Byproducts (MDBP) rules ([U.S. EPA,  
32 2014a](#)).

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## Appendix G

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# Identification and Hazard Evaluation of Chemicals across the Hydraulic Fracturing Water Cycle Supplemental Tables and Information

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*This document is a draft for review purposes only and does not constitute Agency policy.*

## Appendix G. Identification and Hazard Evaluation of Chemicals across the Hydraulic Fracturing Water Cycle Supplemental Tables and Information

1 Appendix G provides detail and supporting information on the oral reference values (RfVs) and oral  
2 slope factors (OSFs) that were identified in Chapter 9 of this assessment.<sup>1</sup> Section G.1 provides  
3 detail on the criteria used to select sources of RfVs and OSFs for chemicals used or detected in  
4 hydraulic fracturing processes, and lists all sources of RfVs and OSFs that were considered for this  
5 study. Section G.2 provides a glossary of the toxicity value terminology that is used by these various  
6 sources. Lastly, all of the RfVs and OSFs collected from these sources are provided in Table G-1 and  
7 Table G-2. Tables G-1a through G-1d show the available RfVs and OSFs for chemicals used in  
8 hydraulic fracturing fluids, and Tables G-2a through G-2d show the available RfVs and OSFs for  
9 chemicals detected in hydraulic fracturing flowback and wastewater. These tables provide cancer  
10 weight-of-evidence (WOE) characterizations for these chemicals where available, and indicate  
11 whether each chemical has available data on physicochemical properties or occurrence.

### G.1. Criteria for Selection and Inclusion of Reference Value (RfV) and Oral Slope Factor (OSF) Data Sources

12 The criteria listed below were used to evaluate the quality of RfVs and OSFs considered for use in  
13 the hazard analyses conducted in Chapter 9. These criteria were originally outlined in the hydraulic  
14 fracturing research plan ([U.S. EPA, 2011a](#)) and interim progress report ([U.S. EPA, 2012c](#)). Only data  
15 sources that met these criteria were considered of sufficient quality to be included in the analyses.

16 The following criteria had to be met for a source to be deemed of sufficient quality:

- 17 1) The body or organization generating or producing the peer-reviewed RfVs, peer-reviewed OSFs,  
18 or peer reviewed qualitative assessment must be a governmental or intergovernmental body.
  - 19 a. Governmental bodies include sovereign states, and federated states/units.
  - 20 b. Intergovernmental bodies are those whose members are sovereign states, and the  
21 subdivisions or agencies of such intergovernmental bodies. The United Nations is an  
22 example of an intergovernmental body. The International Agency for Research on  
23 Cancer (IARC) is an agency of the World Health Organization (WHO), which is itself an  
24 agency of the United Nations. Thus, IARC is considered a subdivision of the United  
25 Nations.

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<sup>1</sup> As defined in Chapter 9, the term RfV refers to reference values for noncancer effects occurring via the oral route of exposure and for chronic durations, except where noted.

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- 1 2) The data source must include peer-reviewed RfVs, peer-reviewed OSFs, or peer reviewed  
2 qualitative assessments.
- 3 a. A committee that is established to derive the RfVs, OSFs, or qualitative assessments can  
4 have members of that same committee provide the peer review, so long as either the  
5 entire committee, or members of the committee who did not participate in the  
6 derivation of a specific section of a work product, conduct the review.
- 7 b. Peer reviewers who work for grantees of the organization deriving the RfVs, OSFs, or  
8 qualitative assessments are generally allowed, and this will not be considered to  
9 constitute a conflict/duality of interest.
- 10 c. Peer reviewers may work in the same or different office, so long as they did not  
11 participate in any way in the development of the product, and these individuals must be  
12 free of conflicts/duality of interest with respect to the chemical(s) assigned.
- 13 i. For instance, peer reviewers for Program X, conducted by Office A, may also be  
14 employed by Office A so long as they did not participate in the creation of the  
15 Program X product they are reviewing.
- 16 3) The RfVs, OSFs, or qualitative assessments must be based on peer-reviewed scientific data.
- 17 a. There are cases where industry reports that were not published in a peer-reviewed,  
18 scholarly journal may be used, if the industry report has been adequately peer-reviewed  
19 by an external body (external to the group generating the report, and external to the  
20 group generating the peer-reviewed RfVs, peer-reviewed OSFs, or peer-reviewed  
21 qualitative assessment) that is free of conflicts/dualities of interest.
- 22 4) The RfVs, OSFs, or qualitative assessments must be focused on protection of the general public.
- 23 a. Sources that are focused on workers are not appropriate as workers are assumed to  
24 accommodate additional risk than the general public due to their status as workers.
- 25 5) The body generating the values or qualitative assessments must be free of conflicts of interest  
26 with respect to the chemicals for which it derives RfVs, OSFs, or qualitative assessments.
- 27 a. If a body generating the RfVs, OSFs, or qualitative assessments accepts funding from an  
28 interested party (i.e., a company or organization that may be impacted by past, present,  
29 or future values or qualitative assessments), then the body has a conflict of interest.
- 30 b. For instance, if a non-profit organization is funded by an industry trade group, and the  
31 non-profit generates RfVs, OSFs, or qualitative assessments for chemicals that trade  
32 group is interested in, then the non-profit is considered to have a conflict of interest  
33 with respect to those chemicals.
- 34 It is important to note that having a conflict/duality of interest for one chemical is sufficient to  
35 disqualify the entire database, as it is assumed that conflicts/dualities of interest may exist for  
36 other chemicals as well.

### G.1.1. Included Sources

1 We applied our criteria to 16 different sources of RfVs and/or OSFs. After application of our criteria,  
2 we were left with eight sources. For those sources which did not meet our criteria, we provide an  
3 explanation of why they were excluded.

4 The following sources were evaluated, met our criteria, and were selected as sources of reference  
5 doses or cancer slope factors for this analysis:

- 6 • **U.S. EPA Integrated Risk Information System (IRIS)**
- 7 • **U.S. EPA Human Health Benchmarks for Pesticides (HHBP)**
- 8 • **U.S. EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs)**
- 9 • **U.S. Agency for Toxic Substances and Disease Registry (ATSDR) Minimum Risk**  
10 **Levels (MRLs)**
- 11 • **California EPA Toxicity Criteria Database**
- 12 • **International Programme On Chemical Safety (IPCS) Concise International Chemical**  
13 **Assessment Documents (CICAD)**

14 The following sources were evaluated, met our criteria, and were selected as sources of qualitative  
15 cancer classifications:

- 16 • **International Agency for Research on Cancer (IARC)**
- 17 • **US National Toxicology Program Report on Carcinogens (RoC)**

18 RfVs and/or OSFs from these data sources are listed in Tables G-1a through G-1d for chemicals used  
19 in hydraulic fracturing fluid formulation, and Tables G-2a through G-2d for chemicals reported in  
20 hydraulic fracturing flowback and produced water.

21 In addition, Table G-1 and Table G-2 also list the EPA's drinking water maximum contaminant levels  
22 (MCLs) and maximum contaminant goal levels (MCLG) when available. These values are generally  
23 based on IRIS values, and are treatment-based. MCL and MCLG values are listed for reference only,  
24 and were not considered in the hazard analysis presented in Chapter 9.

### G.1.2. Excluded Sources

- 25 • **American Conference of Governmental Industrial Hygienists:** The assessments  
26 derived by this body are specific to workers and are not generalizable to the general  
27 public. In addition, this body is not a governmental or intergovernmental body. Thus, these  
28 values were excluded based on criteria 1 and 4.
- 29 • **European Chemicals Bureau, Classification and Labeling Annex I of Directive**  
30 **67/548/EEC:** These assessments are not based on peer-reviewed values, but are based on  
31 data supplied by manufacturers. Further, the enabling legislation states that  
32 "Manufacturers, importers, and downstream users shall examine the information...to  
33 ascertain whether it is adequate, reliable and scientifically valid for the purpose of the

1 evaluation...” This clearly demonstrates that the data and the evaluation are not required  
2 to be peer-reviewed. Thus, these values were excluded based on criterion 2.

- 3 • **Toxicology Excellence for Risk Assessment’s (TERA’s) International Toxicity**  
4 **Estimates for Risk Assessment (ITER):** The ITER database is developed by TERA a  
5 501(c)(3) non-profit. TERA accepts funding from various sources, including interested  
6 parties that may be impacted by their assessment work. Thus, ITER is excluded based on  
7 criteria 1 and 5.
- 8 • **Other U.S. states:** The EPA evaluated values from all states that had values reported on  
9 their websites. If a state’s values were determined to be largely duplicative of the EPA’s  
10 values (e.g., the state adopts EPA values, such as the regional screening levels, and does  
11 not typically generate its own peer-reviewed values), that state’s values were no longer  
12 considered. The EPA contacted those states whose values were determined to not be  
13 duplicative of EPA’s values, and confirmed whether or not a peer review process was used  
14 to develop the state’s values. The EPA determined that of the states with values not  
15 duplicative of the EPA’s values, only California’s values met all of the EPA’s criteria for this  
16 report. Other states with publicly accessible RfVs and/or OSFs include: Alabama, Florida,  
17 Hawaii, and Texas.
- 18 • **WHO Guidelines for Drinking-Water Quality:** The WHO Guidelines’ values are not RfVs,  
19 but rather drinking water values.

## G.2. Glossary of Toxicity Value Terminology

20 This section defines the toxicity values and qualitative cancer classifications that are frequently  
21 found in the sources identified above.

22 **Lowest-observed-adverse-effect level (LOAEL):** The lowest exposure level at which there are  
23 biologically significant increases in frequency or severity of adverse effects between the exposed  
24 population and its appropriate control group. Source: [U.S. EPA \(2011c\)](#).

25 **Maximum allowable daily level (MADL):** The maximum allowable daily level of a reproductive  
26 toxicant at which the chemical would have no observable adverse reproductive effect, assuming  
27 exposure at 1,000 times that level. Source: [OEHHA \(2012\)](#).

28 **Maximum contaminant level (MCL):** The highest level of a contaminant that is allowed in  
29 drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment  
30 technology and taking cost into consideration. MCLs are enforceable standards. Source: [U.S. EPA](#)  
31 [\(2014b\)](#).

32 **Maximum contaminant level goal (MCLG):** The level of a contaminant in drinking water below  
33 which there is no known or expected risk to health. MCLGs allow for a margin of safety and are  
34 nonenforceable public health goals. Source: [U.S. EPA \(2014b\)](#).

35 **Minimum risk level (MRL):** An ATSDR estimate of daily human exposure to a hazardous substance  
36 at or below which the substance is unlikely to pose a measurable risk of harmful (adverse),

1 noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a  
2 specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of  
3 harmful (adverse) health effects.

- 4 • **Chronic MRL:** Duration of exposure is 365 days or longer.
- 5 • **Intermediate MRL:** Duration of exposure is >14 to 364 days.
- 6 • **Acute MRL:** Duration of exposure is 1 to 14 days.

7 Source: [ATSDR \(2009\)](#).

8 **No-observed-adverse-effect level (NOAEL):** The highest exposure level at which there are no  
9 biologically significant increases in the frequency or severity of adverse effect between the exposed  
10 population and its appropriate control; some effects may be produced at this level, but they are not  
11 considered adverse or precursors of adverse effects. Source: [U.S. EPA \(2011c\)](#).

12 **Oral slope factor (OSF):** An upper-bound, approximating a 95% confidence limit, on the increased  
13 cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of  
14 proportion (of a population) affected per mg/kg-day, is generally reserved for use in the low-dose  
15 region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in  
16 100. Source: [U.S. EPA \(2011c\)](#).

17 **Reference dose (RfD) (U.S. EPA IRIS and PPRTV definition):** An estimate (with uncertainty  
18 spanning perhaps an order of magnitude) of a daily oral exposure to the human population  
19 (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects  
20 during a lifetime. It can be derived from a NOAEL, LOAEL, or benchmark dose, with uncertainty  
21 factors generally applied to reflect limitations of the data used. The RfD is generally used in the  
22 EPA's noncancer health assessments.

- 23 • **Chronic RfD:** Duration of exposure is up to a lifetime.
- 24 • **Subchronic RfD (sRfD):** Duration of exposure is up to 10% of an average lifespan.

25 Source: [U.S. EPA \(2011c\)](#).

26 **Reference dose (RfD) (U.S. EPA HHBP definition):** The particular concentration of a chemical  
27 that is known not to cause health problems. A standard that also may be referred to as the  
28 acceptable daily intake. Derived using the same EPA guidance for IRIS and PPRTV RfD  
29 determination. Source: [U.S. EPA \(2015e\)](#).

30 **Tolerable daily intake (TDI):** An estimate of the intake of a substance, expressed on a body mass  
31 basis, to which an individual in a (sub) population may be exposed daily over its lifetime without  
32 appreciable health risk. Source: [WHO \(2015\)](#).

33 **Weight-of-evidence (WOE) characterization for carcinogenicity:** A system used for  
34 characterizing the extent to which the available data support the hypothesis that an agent causes  
35 cancer in humans.

- 1       • **EPA 1986 guidelines:** Under the EPA's 1986 risk assessment guidelines, the WOE was  
2 described by categories "A through E," with Group A for known human carcinogens through  
3 Group E for agents with evidence of noncarcinogenicity. Five standard WOE descriptors  
4 were used:
- 5           ○ A: Human carcinogen
  - 6           ○ B1: Probable human carcinogen—based on limited evidence of carcinogenicity in  
7 humans and sufficient evidence of carcinogenicity in animals
  - 8           ○ B2: Probable human carcinogen—based on sufficient evidence of carcinogenicity in  
9 animals
  - 10          ○ C: Possible human carcinogen
  - 11          ○ D: Not classifiable as to human carcinogenicity
  - 12          ○ E: Evidence of noncarcinogenicity for humans

13       Source: [U.S. EPA \(2011c\)](#).

- 14       • **EPA 1996 proposed guidelines:** The EPA's 1996 proposed guidelines outlined a major  
15 change in the way hazard evidence was weighted in reaching conclusions about the human  
16 carcinogenic potential of agents. These guidelines replaced the WOE letter categories with  
17 the use of standard descriptors of conclusions incorporated into a brief narrative. Three  
18 categories of descriptors with the narrative were used:

- 19           ○ Known/likely
- 20           ○ Cannot be determined
- 21           ○ Not likely

22       Source: [U.S. EPA \(1996\)](#).

- 23       • **EPA 1999 guidelines:** The 1999 guidelines adopted a framework incorporating hazard  
24 identification, dose-response assessment, exposure assessment, and risk characterization  
25 with an emphasis on characterization of evidence and conclusions in each part of the  
26 assessment. Five descriptors summarizing the WOE in the narrative were used:

- 27           ○ Carcinogenic to humans
- 28           ○ Likely to be carcinogenic to humans
- 29           ○ Suggestive evidence of carcinogenicity, but not sufficient to assess human  
30 carcinogenic potential
- 31           ○ Data are inadequate for an assessment of human carcinogenic potential
- 32           ○ Not likely to be carcinogenic to humans

33       Source: [U.S. EPA \(1999\)](#).

- 34       • **EPA 2005 guidelines:** The approach outlined in the EPA's 2005 guidelines for carcinogen  
35 risk assessment considers all scientific information in determining whether and under what  
36 conditions an agent may cause cancer in humans and provides a narrative approach to

1 characterize carcinogenicity rather than categories. Five standard WOE descriptors are  
2 used as part of the narrative:

- 3 ○ Carcinogenic to humans
- 4 ○ Likely to be carcinogenic to humans
- 5 ○ Suggestive evidence of carcinogenic potential
- 6 ○ Inadequate information to assess carcinogenic potential
- 7 ○ Not likely to be carcinogenic to humans

8 Source: [U.S. EPA \(2011c\)](#).

- 9 • **IARC Monographs on the evaluation of carcinogenic risks to humans:** The IARC  
10 classifies carcinogen risk as a matter of scientific judgement that reflects the strength of the  
11 evidence derived from studies in humans, in experimental animals, from mechanistic data,  
12 and from other relevant data. Five WOE classifications are used:

- 13 ○ Group 1: Carcinogenic to humans
- 14 ○ Group 2A: Probably carcinogenic to humans
- 15 ○ Group 2B: Possibly carcinogenic to humans
- 16 ○ Group 3: Not classifiable as to its carcinogenicity to humans
- 17 ○ Group 4: Probably not carcinogenic to humans

18 Source: [IARC \(2015\)](#).

- 19 • **NTP:** The NTP describes the results of individual experiments on a chemical agent and  
20 notes the strength of the evidence for conclusions regarding each study. Negative results, in  
21 which the study animals do not have a greater incidence of neoplasia than control animals,  
22 do not necessarily mean that a chemical is not a carcinogen, inasmuch as the experiments  
23 are conducted under a limited set of conditions. Positive results demonstrate that a  
24 chemical is carcinogenic for laboratory animals under the conditions of the study and  
25 indicate that exposure to the chemical has the potential for hazard to humans. For each  
26 separate experiment, one of the following five categories is selected to describe the findings.  
27 These categories refer to the strength of the experimental evidence and not to potency or  
28 mechanism.

- 29 ○ Clear evidence of carcinogenic activity
- 30 ○ Some evidence of carcinogenic activity
- 31 ○ Equivocal evidence of carcinogenic activity
- 32 ○ No evidence of carcinogenic activity
- 33 ○ Inadequate study of carcinogenic activity

34 Source: [NTP \(2014a\)](#).

- 35 • **The RoC** is a congressionally mandated, science-based, public health report that identifies  
36 agents, substances, mixtures, or exposures (collectively called “substances”) in our

1 environment that may potentially put people in the United States at increased risk for  
2 cancer. NTP prepares the RoC on behalf of the Secretary of the Health and Human Services.  
3 The listing criteria in the RoC Document are:

- 4       ○ Known to be a human carcinogen
- 5       ○ Reasonably anticipated to be a human carcinogen

6 Source: [NTP \(2014b\)](#).

### G.3. Tables

**Table G-1a. Chemicals reported to be used in hydraulic fracturing fluids, with available federal chronic RfVs and OSFs.**

Chemicals from the FracFocus database are listed first, ranked by IRIS reference dose (RfD). The “--” symbol indicates that no value was available from the sources consulted. Additionally, an “x” indicates the availability of usage data from FracFocus ([U.S. EPA, 2015a](http://www.fracfocus.com)) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic oral MRL <sup>d</sup> (mg/kg-day)	Chronic RfD <sup>e</sup> (mg/kg-day)	Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
Acrylamide	79-06-1	x	x	0.002	0.5	"Likely to be carcinogenic to humans"	--	--	--	0.001	--	0	--
Propargyl alcohol	107-19-7	x	x	0.002	--	--	--	--	--	--	--	--	--
Furfural	98-01-1	x	x	0.003	--	--	--	--	--	--	0.01	--	--
<i>Benzene</i>	<i>71-43-2</i>	x	x	<i>0.004</i>	<i>0.015-0.055</i>	<i>A</i>	--	--	--	<i>0.0005</i>	--	<i>0</i>	<i>0.005</i>
<i>Dichloromethane</i>	<i>75-09-2</i>	x	x	<i>0.006</i>	<i>0.002</i>	<i>"Likely to be carcinogenic in humans"</i>	--	--	--	<i>0.06</i>	--	<i>0</i>	<i>0.005</i>
<i>Naphthalene</i>	<i>91-20-3</i>	x	x	<i>0.02</i>	--	<i>"Data are inadequate to assess human carcinogenic potential"</i>	--	--	--	--	--	--	--

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Chemical Name	CASRN	Frac-Focus data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic oral MRL <sup>d</sup> (mg/kg-day)	Chronic RfD <sup>e</sup> (mg/kg-day)	Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
1,4-Dioxane	123-91-1	x	x	0.03	0.1	"Likely to be carcinogenic to humans"	--	--	--	0.1	--	--	--
Sodium chlorite	7758-19-2	x		0.03	--	"Data are inadequate to assess human carcinogenicity"	--	--	--	--	--	1	0.8
Chlorine dioxide	10049-04-4	x		0.03	--	"Data are inadequate to assess human carcinogenicity"	--	--	--	--	--	--	--
1,3-Dichloropropene	542-75-6	x	x	0.03	0.05	"Likely to be a human carcinogen"	--	--	--	0.03	--	--	--
Bisphenol A	80-05-7	x	x	0.05	--	--	--	--	--	--	--	--	--
Toluene	108-88-3	x	x	0.08	--	"Inadequate information to assess the carcinogenic potential"	--	--	--	--	--	1	1
Ethylbenzene	100-41-4	x	x	0.1	--	D	--	--	--	--	--	0.7	0.7

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				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic oral MRL <sup>d</sup> (mg/kg-day)	Chronic RfD <sup>e</sup> (mg/kg-day)	Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
1-Butanol	71-36-3	x	x	0.1	--	D	--	--	--	--	--	--	--
<i>Cumene</i>	98-82-8	x	x	0.1	--	D	--	--	--	--	--	--	--
<i>Acetophenone</i>	98-86-2	x	x	0.1	--	D	--	--	--	--	--	--	--
2-Butoxyethanol	111-76-2	x	x	0.1	--	"Not likely to be carcinogenic to humans"	--	--	--	--	--	--	--
<i>Xylenes</i>	1330-20-7	x	x	0.2	--	"Data are inadequate to assess the carcinogenic potential"	--	--	--	0.2	--	10	10
Formaldehyde	50-00-0	x	x	0.2	--	B1	--	--	--	0.2	--	--	--
<i>Phenol</i>	108-95-2	x	x	0.3	--	"Data are inadequate for an assessment of human carcinogenic potential"	--	--	--	--	--	--	--
2-Methyl-1-propanol	78-83-1	x	x	0.3	--	--	--	--	--	--	--	--	--

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				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic oral MRL <sup>d</sup> (mg/kg-day)	Chronic RfD <sup>e</sup> (mg/kg-day)	Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
Acetone	67-64-1	x	x	0.9	--	"Data are inadequate for an assessment of human carcinogenic potential"	--	--	--	--	--	--	--
Ethyl acetate	141-78-6	x	x	0.9	--	--	--	--	IN	--	--	--	--
Ethylene glycol	107-21-1	x	x	2	--	--	--	--	--	--	--	--	--
Methanol	67-56-1	x	x	2	--	--	--	--	--	--	--	--	--
Benzoic acid	65-85-0	x	x	4	--	D	--	--	--	--	--	--	--
Aniline	62-53-3	x	x	--	0.0057	B2	0.007	--	--	--	--	--	--
Benzyl chloride	100-44-7	x	x	--	0.17	B2	0.002	--	--	--	--	--	--
(E)-Crotonaldehyde	123-73-9	x	x	--	--	C	0.001	--	--	--	--	--	--
N,N-Dimethylformamide	68-12-2	x	x	--	--	--	0.1	--	IN	--	--	--	--
Epichlorohydrin	106-89-8	x	x	--	0.0099	B2	0.006	--	--	--	--	0	--
1,2-Propylene glycol	57-55-6	x	x	--	--	--	20	--	NL	--	--	--	--

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2-(2-Butoxyethoxy) ethanol	112-34-5	x	x	--	--	--	0.03	--	IN	--	--	--	--
Hexanedioic acid	124-04-9	x	x	--	--	--	2	--	--	--	--	--	--
Quinoline	91-22-5	x	x	--	3	"Likely to be carcinogenic in humans"	--	--	--	--	--	--	--
Ethylenediamine	107-15-3	x	x	--	--	D	0.09	--	IN	--	--	--	--
<i>Formic acid</i>	<i>64-18-6</i>	x	x	--	--	--	<i>0.9</i>	--	<i>IN</i>	--	--	--	--
Sodium chlorate	7775-09-9	x		--	--	--	--	--	--	--	0.03	--	--
Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	68424-85-1	x		--	--	--	--	--	--	--	0.44	--	--
Benzenesulfonic acid, C10-16-alkyl derivs.	68584-22-5	x		--	--	--	--	--	--	--	0.5	--	--
Ammonium phosphate	7722-76-1	x		--	--	--	49	--	IN	--	--	--	--
Didecyldimethylammonium chloride	7173-51-5	x	x	--	--	--	--	--	--	--	0.1	--	--
2-(Thiocyanomethylthio)benzotriazole	21564-17-0	x	x	--	--	--	--	--	--	--	0.01	--	--

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Mineral oil - includes paraffin oil	8012-95-1	x		--	--	--	3	--	IN	--	--	--	--
Trisodium phosphate	7601-54-9	x		--	--	--	49	--	IN	--	--	--	--
Triphosphoric acid, pentasodium salt	7758-29-4	x		--	--	--	49	--	IN	--	--	--	--
<i>Aluminum</i>	7429-90-5	x		--	--	--	1	--	IN	1	--	--	--
Phosphoric acid	7664-38-2	x		--	--	--	48.6	--	IN	--	--	--	--
<i>Iron</i>	7439-89-6	x		--	--	--	0.7	--	IN	--	--	--	--
Tricalcium phosphate	7758-87-4	x		--	--	--	49	--	IN	--	--	--	--
<i>Bis(2-chloroethyl) ether</i>	111-44-4	x	x	--	1.1	B2	--	--	--	--	--	--	--
Dodecylbenzenesulfonic acid	27176-87-0	x	x	--	--	--	--	--	--	--	0.5	--	--
Hydrazine	302-01-2	x		--	3	B2	--	--	--	--	--	--	--
Tetrasodium pyrophosphate	7722-88-5	x		--	--	--	49	--	IN	--	--	--	--

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Potassium phosphate, tribasic	7778-53-2	x		--	--	--	49	--	IN	--	--	--	--
Sodium trimetaphosphate	7785-84-4	x		--	--	--	49	--	IN	--	--	--	--
Arsenic	7440-38-2			0.0003	1.5	A	--	--	--	0.0003	--	0	0.010
Phosphine	7803-51-2			0.0003	--	D	--	--	--	--	--	--	--
Acrolein	107-02-8		x	0.0005	--	"Data are inadequate for an assessment of human carcinogenic potential"	--	--	--	--	--	--	--
Chromium (VI)	18540-29-9			0.003	--	A (inhaled); D(oral)	--	--	--	0.0009	--	--	--
Di(2-ethylhexyl) phthalate	117-81-7		x	0.02	0.014	B2	--	--	--	0.06	--	0	0.006
Chlorine	7782-50-5			0.1	--	--	--	--	--	--	--	--	--
Styrene	100-42-5		x	0.2	--	--	--	--	--	--	--	0.1	0.1

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Zinc	7440-66-6			0.3	--	"Inadequate information to assess carcinogenic potential"	--	--	--	0.3	--	--	--
Acrylic acid	79-10-7		x	0.5	--	--	--	--	IN	--	--	--	--
Chromium (III)	16065-83-1			1.5	--	"Data are inadequate for an assessment of human carcinogenic potential"	--	--	--	--	--	--	--
Phthalic anhydride	85-44-9		x	2	--	--	--	--	--	--	--	--	--
Cyclohexanone	108-94-1		x	5	--	--	--	--	IN	--	--	--	--
1,2-Propylene oxide	75-56-9		x	--	0.24	B2	--	--	--	--	0.001	--	--
2-(2-Ethoxyethoxy) ethanol	111-90-0		x	--	--	--	0.06	--	IN	--	--	--	--
Tributyl phosphate	126-73-8		x	--	--	--	0.01	0.009	LI	0.08	--	--	--
2-Methoxyethanol	109-86-4		x	--	--	--	0.005	--	IN	--	--	--	--
Polyphosphoric acids, sodium salts	68915-31-1			--	--	--	49	--	IN	--	--	--	--
Phosphoric acid, diammonium salt	7783-28-0			--	--	--	49	--	IN	--	--	--	--

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Sodium pyrophosphate	7758-16-9			--	--	--	49	--	IN	--	--	--	--
Phosphoric acid, aluminium sodium salt	7785-88-8			--	--	--	49	--	IN	--	--	--	--

ATSDR = Agency for Toxic Substances and Disease Registry; CASRN = Chemical Abstract Service Registry Number; IRIS = Integrated Risk Information System; PPRTV = Provisional Peer Reviewed Toxicity Values; HHBP = Human Health Benchmarks for Pesticides

<sup>a</sup> Reference dose (RfD) (IRIS and PPRTV definition): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Chronic RfD: Duration of exposure is up to a lifetime.

<sup>b</sup> Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg-day, is generally reserved for use in the low dose region of the dose response relationship, that is, for exposures corresponding to risks less than 1 in 100.

<sup>c</sup> Weight of evidence (WOE) characterization for carcinogenicity: A system used for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. See glossary for details.

<sup>d</sup> Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Chronic MRL: Duration of exposure is 365 days or longer.

<sup>e</sup> Reference dose (RfD) (HHBP definition): The particular concentration of a chemical that is known not to cause health problems. A standard that also may be referred to as the acceptable daily intake. Derived using the same EPA guidance for RfD determination.

<sup>f</sup> Maximum contaminant level goal (MCLG): The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are nonenforceable public health goals.

<sup>g</sup> Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards.

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**Table G-1b. Chemicals reported to be used in hydraulic fracturing fluids, with available state chronic RfVs and OSFs.**

Chemicals from the FracFocus database are listed first, ranked by California EPA maximum allowable daily level (MADL). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of usage data from FracFocus ([U.S. EPA, 2015a](#)) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	California	
				Oral MADL <sup>a</sup> (µg/day)	OSF <sup>b</sup> (per mg/kg-day)
Ethylene oxide	75-21-8	x	x	20	0.31
<i>Benzene</i>	<i>71-43-2</i>	x	x	24	<i>0.1</i>
N-Methyl-2-pyrrolidone	872-50-4	x	x	17000	--
Acrylamide	79-06-1	x	x	140	4.5
Aniline	62-53-3	x	x	--	0.0057
Benzyl chloride	100-44-7	x	x	--	0.17
<i>1,4-Dioxane</i>	<i>123-91-1</i>	x	x	--	<i>0.027</i>
Epichlorohydrin	106-89-8	x	x	--	0.08
<i>Ethylbenzene</i>	<i>100-41-4</i>	x	x	--	<i>0.011</i>
Nitrilotriacetic acid	139-13-9	x	x	--	0.0053
Nitrilotriacetic acid trisodium monohydrate	18662-53-8	x	x	--	0.01
Thiourea	62-56-6	x	x	--	0.072
<i>Bis(2-chloroethyl) ether</i>	<i>111-44-4</i>	x	x	--	<i>2.5</i>
1,3-Butadiene	106-99-0	x	x	--	0.6
Hydrazine	302-01-2	x		--	3
1,3-Dichloropropene	542-75-6	x	x	--	0.091
<i>Dichloromethane</i>	<i>75-09-2</i>	x	x	--	<i>0.014</i>
<i>Lead</i>	<i>7439-92-1</i>			<i>0.5</i>	<i>0.0085</i>
<i>Chromium (VI)</i>	<i>18540-29-9</i>			<i>8.2</i>	<i>0.5</i>
2-Methoxyethanol	109-86-4		x	63	--
2-Ethoxyethanol	110-80-5		x	750	--

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Chemical name	CASRN	FracFocus data available	Physico-chemical data available	California	
				Oral MADL <sup>a</sup> (µg/day)	OSF <sup>b</sup> (per mg/kg-day)
<i>Di(2-ethylhexyl) phthalate</i>	117-81-7		x	20 (neonate male) 58 (infant male) 410 (adult)	0.003
1,2-Propylene oxide	75-56-9		x	--	0.24
<i>Arsenic</i>	7440-38-2			--	9.5

<sup>a</sup> Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level.

<sup>b</sup> Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100.

**Table G-1c. Chemicals reported to be used in hydraulic fracturing fluids, with available international chronic RfVs and OSFs.**

Chemicals from the FracFocus database are listed first, ranked by CICAD reference dose (TDI, or tolerable daily intake). An “x” indicates the availability of usage data from FracFocus ([U.S. EPA, 2015a](https://www.epa.gov/fracfocus)) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physicochemical data available	IPCS Chronic TDI <sup>a</sup> (mg/kg-day)
D-Limonene	5989-27-5	x	x	0.1
Potassium iodide	7681-11-0	x		0.01
Sodium iodide	7681-82-5	x		0.01
Copper(I) iodide	7681-65-4	x		0.01
Glyoxal	107-22-2	x	x	0.2
<i>Ethylene glycol</i>	<i>107-21-1</i>	x	x	<i>0.05</i>
N-Methyl-2-pyrrolidone	872-50-4	x	x	0.6
Strontium chloride	10476-85-4			0.13
<i>Chromium (VI)</i>	<i>18540-29-9</i>			<i>0.0009</i>

IPCS = International Programme on Chemical Safety; CICAD = Concise International Chemical Assessment Documents

<sup>a</sup> Tolerable daily intake (TDI): An estimate of the intake of a substance, expressed on a body mass basis, to which an individual in a (sub) population may be exposed daily over its lifetime without appreciable health risk.

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**Table G-1d. Chemicals reported to be used in hydraulic fracturing fluids, with available less-than-chronic RfVs and OSFs.**

Chemicals from the FracFocus database are listed first, ranked by PPRTV subchronic reference dose (sRfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of usage data from FracFocus ([U.S. EPA, 2015a](#)) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD <sup>a</sup> (mg/kg-day)	Acute oral MRL <sup>b</sup> (mg/kg-day)	Intermediate oral MRL <sup>c</sup> (mg/kg-day)
Benzyl chloride	100-44-7	x	x	0.002	--	--
Epichlorohydrin	106-89-8	x	x	0.006	--	--
(E)-Crotonaldehyde	123-73-9	x	x	0.01	--	--
<i>Benzene</i>	<i>71-43-2</i>	x	x	<i>0.01</i>	--	--
<i>Ethylbenzene</i>	<i>100-41-4</i>	x	x	<i>0.05</i>	--	<i>0.4</i>
Ethylenediamine	107-15-3	x	x	0.2	--	--
N,N-Dimethylformamide	68-12-2	x	x	0.3	--	--
2-(2-Butoxyethoxy)ethanol	112-34-5	x	x	0.3	--	--
Hexane	110-54-3	x	x	0.3	--	--
<i>Xylenes</i>	<i>1330-20-7</i>	x	x	<i>0.4</i>	<i>1</i>	<i>0.4</i>
Antimony trioxide	1309-64-4	x		0.5	--	--
<i>Iron</i>	<i>7439-89-6</i>	x		<i>0.7</i>	--	--
<i>Toluene</i>	<i>108-88-3</i>	x	x	<i>0.8</i>	<i>0.8</i>	<i>0.02</i>
<i>Formic acid</i>	<i>64-18-6</i>	x	x	<i>0.9</i>	--	--
Hexanedioic acid	124-04-9	x	x	2	--	--
Benzoic acid	65-85-0	x	x	4	--	--
<i>1,2-Propylene glycol</i>	<i>57-55-6</i>	x	x	<i>20</i>	--	--
Mineral oil - includes paraffin oil	8012-95-1	x		30	--	--
Phosphoric acid	7664-38-2	x		48.6	--	--
Ammonium phosphate	7722-76-1	x		49	--	--
Trisodium phosphate	7601-54-9	x		49	--	--
Triphosphoric acid, pentasodium salt	7758-29-4	x		49	--	--

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Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD <sup>a</sup> (mg/kg-day)	Acute oral MRL <sup>b</sup> (mg/kg-day)	Intermediate oral MRL <sup>c</sup> (mg/kg-day)
Tricalcium phosphate	7758-87-4	x		49	--	--
Tetrasodium pyrophosphate	7722-88-5	x		49	--	--
Potassium phosphate, tribasic	7778-53-2	x		49	--	--
Sodium trimetaphosphate	7785-84-4	x		49	--	--
Acrylamide	79-06-1	x	x	--	0.01	0.001
<i>1,4-Dioxane</i>	<i>123-91-1</i>	x	x	--	5	0.5
<i>Ethylene glycol</i>	<i>107-21-1</i>	x	x	--	0.8	0.8
<i>Naphthalene</i>	<i>91-20-3</i>	x	x	--	0.6	0.6
<i>Phenol</i>	<i>108-95-2</i>	x	x	--	1	--
Sodium chlorite	7758-19-2	x		--	--	0.1
<i>Acetone</i>	<i>67-64-1</i>	x	x	--	--	2
2-Butoxyethanol	111-76-2	x	x	--	0.4	0.07
<i>Aluminum</i>	<i>7429-90-5</i>	x		--	--	1
Formaldehyde	50-00-0	x	x	--	--	0.3
1,3-Dichloropropene	542-75-6	x	x	--	--	0.04
<i>Dichloromethane</i>	<i>75-09-2</i>	x	x	--	0.2	--
Antimony trichloride	10025-91-9			0.0004	--	--
2-Methoxyethanol	109-86-4		x	0.02	--	--
Tributyl phosphate	126-73-8		x	0.03	1.1	0.08
Acrylic acid	79-10-7		x	0.2	--	--
2-(2-Ethoxyethoxy) ethanol	111-90-0		x	0.6	--	--
Cyclohexanone	108-94-1		x	2	--	--
Polyphosphoric acids, sodium salts	68915-31-1			49	--	--
Phosphoric acid, diammonium salt	7783-28-0			49	--	--
Sodium pyrophosphate	7758-16-9			49	--	--

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Chemical name	CASRN	FracFocus data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD <sup>a</sup> (mg/kg-day)	Acute oral MRL <sup>b</sup> (mg/kg-day)	Intermediate oral MRL <sup>c</sup> (mg/kg-day)
Phosphoric acid, aluminium sodium salt	7785-88-8			49	--	--
<i>Acrolein</i>	107-02-8		x	--	--	0.004
<i>Di(2-ethylhexyl) phthalate</i>	117-81-7		x	--	--	0.1
Styrene	100-42-5		x	--	0.1	--
<i>Arsenic</i>	7440-38-2			--	0.005	--
<i>Chromium (VI)</i>	18540-29-9			--	--	0.005
<i>Copper</i>	7440-50-8			--	0.01	0.01
<i>Zinc</i>	7440-66-6			--	--	0.3

<sup>a</sup> Reference dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Subchronic RfD (sRfD): Duration of exposure is up to 10% of an average lifespan.

<sup>b</sup> Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Acute MRL: Duration of exposure is 1 to 14 days.

<sup>c</sup> Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Intermediate MRL: Duration of exposure is >14 to 364 days.

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**Table G-2a. Chemicals reported to be detected in flowback or produced water, with available federal chronic RfVs and OSFs.**

Chemicals are ranked by IRIS reference dose (RfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical Name	CASRN	Concentration data available	Physicochemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic oral MRL <sup>d</sup> (mg/kg-day)	Chronic RfD <sup>e</sup> (mg/kg-day)	Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
Heptachlor epoxide	1024-57-3		x	0.000013	9.1	B2	--	--	--	--	--	0	0.0002
Phosphorus	7723-14-0	x		0.00002	--	D	--	--	--	--	--	--	--
Aldrin	309-00-2		x	0.00003	17	B2	--	--	--	0.00003	--	--	--
Dieldrin	60-57-1		x	0.00005	16	B2	--	--	--	0.00005	--	--	--
<i>Arsenic</i>	<i>7440-38-2</i>	x		<i>0.0003</i>	<i>1.5</i>	<i>A</i>	--	--	--	<i>0.0003</i>	--	<i>0</i>	<i>0.010</i>
Lindane	58-89-9		x	0.0003	--	--	--	--	--	--	--	0.0002	0.0002
Antimony	7440-36-0	x		0.0004	--	--	--	--	IN	--	--	0.006	0.006
<i>Acrolein</i>	<i>107-02-8</i>		x	<i>0.0005</i>	--	<i>"Data are inadequate for an assessment of human carcinogenic potential"</i>	--	--	--	--	--	--	--
Cadmium	7440-43-9	x		0.0005 (water)	--	B1	--	--	--	0.0001	--	0.005	0.005
Heptachlor	76-44-8		x	0.0005	4.5	B2	--	--	--	--	--	0	0.0004

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Chemical Name	CASRN	Concentration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR Chronic oral MRL <sup>d</sup> (mg/kg-day)	HHBP Chronic RfD <sup>e</sup> (mg/kg-day)	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>			Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
Cyanide	57-12-5		x	0.0006	--	"Inadequate information to assess the carcinogenic potential"	--	--	--	--	--	0.2	0.2
Pyridine	110-86-1	x	x	0.001	--	--	--	--	--	--	--	--	--
Methyl bromide	74-83-9		x	0.0014	--	D	--	--	--	--	0.02	--	--
Beryllium	7440-41-7	x		0.002	--	B1	--	--	--	0.002	--	0.004	0.004
Chromium (VI)	18540-29-9			0.003	--	A (inhaled); D(oral)	--	--	--	0.0009	--	--	--
Benzene	71-43-2	x	x	0.004	0.015-0.055	A	--	--	--	0.0005	--	0	0.005
2-Methylnaphthalene	91-57-6	x	x	0.004	--	"Data are inadequate to assess human carcinogenic potential"	--	--	--	0.04	--	--	--
Molybdenum	7439-98-7	x		0.005	--	--	--	--	--	--	--	--	--
Silver	7440-22-4	x		0.005	--	D	--	--	--	--	--	--	--
Selenium	7782-49-2	x		0.005	--	D	--	--	--	0.005	--	0.05	0.05
Dichloromethane	75-09-2		x	0.006	0.002	"Likely to be carcinogenic in humans"	--	--	--	0.06	--	0	0.005

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Chemical Name	CASRN	Concentration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR Chronic oral MRL <sup>d</sup> (mg/kg-day)	HHBP Chronic RfD <sup>e</sup> (mg/kg-day)	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>			Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
1,2,4-Trichlorobenzene	120-82-1		x	0.01	--	D	--	0.029	LI	0.1	--	0.07	0.07
Tetrachloroethylene	127-18-4		x	0.006	0.0021	"Likely to be carcinogenic in humans"	--	--	--	0.008	--	0	0.005
Chloroform	67-66-3	x	x	0.01	--	B2	--	--	--	0.01	--	--	--
<i>Di(2-ethylhexyl) phthalate</i>	117-81-7	x	x	0.02	0.014	B2	--	--	--	0.06	--	0	0.006
<i>Naphthalene</i>	91-20-3	x	x	0.02	--	"Data are inadequate to assess human carcinogenic potential"	--	--	--	--	--	--	--
2,4-Dimethylphenol	105-67-9	x	x	0.02	--	--	--	--	IN	--	--	--	--
Chlorodibromomethane	124-48-1		x	0.02	0.084	C	--	--	--	0.09	--	--	--
Bromoform	75-25-2		x	0.02	0.0079	B2	--	--	--	0.02	--	--	--
Bromodichloromethane	75-27-4		x	0.02	0.062	B2	--	--	--	0.02	--	--	--
Diphenylamine	122-39-4	x	x	0.025	--	--	--	--	IN	--	0.1	--	--
<i>1,4-Dioxane</i>	123-91-1	x	x	0.03	0.1	"Likely to be carcinogenic to humans"	--	--	--	0.1	--	--	--

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Chemical Name	CASRN	Concentration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR Chronic oral MRL <sup>d</sup> (mg/kg-day)	HHBP Chronic RfD <sup>e</sup> (mg/kg-day)	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>			Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
Pyrene	129-00-0	x	x	0.03	--	D	--	--	--	--	--	--	--
Fluoranthene	206-44-0	x	x	0.04	--	D	--	--	IN	--	--	--	--
Fluorene	86-73-7	x	x	0.04	--	D	--	--	--	--	--	--	--
m-Cresol	108-39-4	x	x	0.05	--	C	--	--	--	--	--	--	--
o-Cresol	95-48-7	x	x	0.05	--	C	--	--	IN	--	--	--	--
<i>Toluene</i>	<i>108-88-3</i>	<i>x</i>	<i>x</i>	<i>0.08</i>	<i>--</i>	<i>"Inadequate information to assess the carcinogenic potential"</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>1</i>	<i>1</i>
<i>Chlorine</i>	<i>7782-50-5</i>			<i>0.1</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>
<i>Ethylbenzene</i>	<i>100-41-4</i>	<i>x</i>	<i>x</i>	<i>0.1</i>	<i>--</i>	<i>D</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>0.7</i>	<i>0.7</i>
<i>Cumene</i>	<i>98-82-8</i>	<i>x</i>	<i>x</i>	<i>0.1</i>	<i>--</i>	<i>D</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>
<i>Acetophenone</i>	<i>98-86-2</i>	<i>x</i>	<i>x</i>	<i>0.1</i>	<i>--</i>	<i>D</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>	<i>--</i>
Carbon disulfide	75-15-0	x	x	0.1	--	--	--	--	--	--	--	--	--
Dibutyl phthalate	84-74-2	x	x	0.1	--	D	--	--	--	--	--	--	--

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Chemical Name	CASRN	Concentration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR Chronic oral MRL <sup>d</sup> (mg/kg-day)	HHBP Chronic RfD <sup>e</sup> (mg/kg-day)	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>			Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
Nitrite	14797-65-0	x		0.1	--	--	--	--	--	--	--	1	1
Manganese	7439-96-5	x		0.14	--	D	--	--	--	--	--	--	--
Xylenes	1330-20-7	x	x	0.2	--	"Data are inadequate to assess the carcinogenic potential"	--	--	--	0.2	--	10	10
Barium	7440-39-3	x		0.2	--	"Not likely to be carcinogenic to humans"	--	--	--	0.2	--	2	2
Boron	7440-42-8	x		0.2	--	"Data are inadequate to assess the carcinogenic potential"	--	--	--	--	--	--	--
Zinc	7440-66-6	x		0.3	--	"Inadequate information to assess carcinogenic potential"	--	--	--	0.3	--	--	--
Phenol	108-95-2	x	x	0.3	--	"Data are inadequate to assess human carcinogenicity"	--	--	--	--	--	--	--

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Chemical Name	CASRN	Concentration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR Chronic oral MRL <sup>d</sup> (mg/kg-day)	HHBP Chronic RfD <sup>e</sup> (mg/kg-day)	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>			Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
Strontium	7440-24-6	x		0.6	--	--	--	--	--	--	--	--	--
Methyl ethyl ketone	78-93-3		x	0.6	--	"Data are inadequate to assess carcinogenic potential"	--	--	--	--	--	--	--
Diethyl phthalate	84-66-2		x	0.8	--	D	--	--	--	--	--	--	--
Acetone	67-64-1	x	x	0.9	--	"Data are inadequate to assess human carcinogenicity"	--	--	--	--	--	--	--
Chromium (III)	16065-83-1			1.5	--	"Data are inadequate to assess human carcinogenicity"	--	--	--	--	--	--	--
Nitrate	14797-55-8	x		1.6	--	--	--	--	--	--	--	10	10
Ethylene glycol	107-21-1		x	2	--	--	--	--	--	--	--	--	--
Methanol	67-56-1		x	2	--	--	--	--	--	--	--	--	--
1,2-Propylene glycol	57-55-6		x	--	--	--	20	--	NL	--	--	--	--
Formic acid	64-18-6		x	--	--	--	0.9	--	IN	--	--	--	--
Aluminum	7429-90-5	x		--	--	--	1	--	IN	1	--	--	--

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Chemical Name	CASRN	Concentration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic oral MRL <sup>d</sup> (mg/kg-day)	Chronic RfD <sup>e</sup> (mg/kg-day)	Public health goal <sup>f</sup> (MCLG) (mg/L)	MCL <sup>g</sup> (mg/L)
Iron	7439-89-6	x		--	--	--	0.7	--	IN	--	--	--	--
Bis(2-chloroethyl) ether	111-44-4		x	--	1.1	B2	--	--	--	--	--	--	--
Benzyl alcohol	100-51-6	x	x	--	--	--	0.1	--	IN	--	--	--	--
Butylbenzene	104-51-8		x	--	--	--	0.05	--	IN	--	--	--	--
Acrylonitrile	107-13-1		x	--	0.54	B1	--	--	--	0.04	--	--	--
Phorate	298-02-2		x	--	--	--	--	--	--	--	0.0005	--	--
beta-Hexachloro cyclohexane	319-85-7		x	--	1.8	C	--	--	--	--	--	--	--
Benzo(a)pyrene	50-32-8	x	x	--	7.3	B2	--	--	--	--	--	0	0.0002
p,p'-DDE	72-55-9		x	--	0.34	B2	--	--	--	--	--	--	--
Lithium	7439-93-2	x		--	--	--	0.002	--	IN	--	--	--	--

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Chemical Name	CASRN	Concentration data available	Physico-chemical data available	IRIS			PPRTV			ATSDR	HHBP	National Primary Drinking Water Regulations	
				Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>	Chronic RfD <sup>a</sup> (mg/kg-day)	OSF <sup>b</sup> (per mg/kg-day)	Cancer WOE characterization <sup>c</sup>			Chronic oral MRL <sup>d</sup> (mg/kg-day)	Chronic RfD <sup>e</sup> (mg/kg-day)
Cobalt	7440-48-4	x		--	--	--	0.0003	--	LI	--	--	--	--
Vanadium	7440-62-2	x		--	--	--	0.00007	--	IN	--	--	--	--
N-Nitrosodiphenylamine	86-30-6	x	x	--	0.0049	B2	--	--	--	--	--	--	--

ATSDR = Agency for Toxic Substances and Disease Registry; CASRN = Chemical Abstract Service Registry Number; IRIS = Integrated Risk Information System; PPRTV = Provisional Peer Reviewed Toxicity Values; HHBP = Human Health Benchmarks for Pesticides

<sup>a</sup> Reference dose (RfD) (IRIS and PPRTV definition): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Chronic RfD: Duration of exposure is up to a lifetime.

<sup>b</sup> Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low dose region of the dose response relationship, that is, for exposures corresponding to risks less than 1 in 100.

<sup>c</sup> Weight of evidence (WOE) characterization for carcinogenicity: A system used for characterizing the extent to which the available data support the hypothesis that an agent causes cancer in humans. See glossary for details.

<sup>d</sup> Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Chronic MRL: Duration of exposure is 365 days or longer.

<sup>e</sup> Reference dose (RfD) (HHBP definition): The particular concentration of a chemical that is known not to cause health problems. A standard that also may be referred to as the acceptable daily intake. Derived using the same EPA guidance for RfD determination.

<sup>f</sup> Maximum contaminant level goal (MCLG): The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are nonenforceable public health goals.

<sup>g</sup> Maximum contaminant level (MCL): The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards.

**Table G-2b. Chemicals reported to be detected in flowback or produced water, with available state chronic RfVs and OSFs.**

Chemicals are ranked by California EPA maximum allowable daily level (MADL). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concentration data available	Physico-chemical data available	California	
				Oral MADL <sup>a</sup> (µg/day)	OSF <sup>b</sup> (per mg/kg-day)
<i>Lead</i>	7439-92-1	x		0.5	0.0085
Cadmium	7440-43-9	x		4.1	15
<i>Chromium (VI)</i>	18540-29-9			8.2	0.5
Dibutyl phthalate	84-74-2	x	x	8.7	--
<i>Benzene</i>	71-43-2	x	x	24	0.1
Acrylonitrile	107-13-1		x	--	1
<i>1,4-Dioxane</i>	123-91-1	x	x	--	0.027
<i>Ethylbenzene</i>	100-41-4	x	x	--	0.011
<i>Di(2-ethylhexyl) phthalate</i>	117-81-7	x	x	20 (neonate male) 58 (infant male) 410 (adult)	0.003
<i>Arsenic</i>	7440-38-2	x		--	9.5
<i>Bis(2-chloroethyl) ether</i>	111-44-4		x	--	2.5
Heptachlor epoxide	1024-57-3		x	--	5.5
1,2,4-Trichlorobenzene	120-82-1		x	--	0.0036
Tetrachloroethylene	127-18-4		x	--	0.051
Indeno(1,2,3-cd)pyrene	193-39-5	x	x	--	1.2
Benzo(b)fluoranthene	205-99-2	x	x	--	1.2
Benzo(k)fluoranthene	207-08-9	x	x	--	1.2
Aldrin	309-00-2		x	--	17
beta-Hexachlorocyclohexane	319-85-7		x	--	1.5
Benzo(a)pyrene	50-32-8	x	x	--	2.9
Dibenz(a,h)anthracene	53-70-3	x	x	--	4.1
7,12-Dimethylbenz(a)anthracene	57-97-6		x	--	250
Lindane	58-89-9		x	--	1.1
Dieldrin	60-57-1		x	--	16
Chloroform	67-66-3	x	x	--	0.019

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Chemical name	CASRN	Concentration data available	Physico-chemical data available	California	
				Oral MADL <sup>a</sup> (µg/day)	OSF <sup>b</sup> (per mg/kg-day)
p,p'-DDE	72-55-9		x	--	0.34
Bromoform	75-25-2		x	--	0.011
Bromodichloromethane	75-27-4		x	--	0.13
Heptachlor	76-44-8		x	--	4.1
N-Nitrosodiphenylamine	86-30-6	x	x	--	0.009
Safrole	94-59-7		x	--	0.22
<i>Dichloromethane</i>	<i>75-09-2</i>		x	--	<i>0.014</i>

<sup>a</sup> Maximum allowable daily level (MADL): The maximum allowable daily level of a reproductive toxicant at which the chemical would have no observable adverse reproductive effect, assuming exposure at 1,000 times that level.

<sup>b</sup> Oral slope factor (OSF): An upper-bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of proportion (of a population) affected per mg/kg day, is generally reserved for use in the low-dose region of the dose-response relationship, that is, for exposures corresponding to risks less than 1 in 100.

**Table G-2c. Chemicals reported to be detected in flowback or produced water, with available international chronic RfVs and OSFs.**

Chemicals are ranked by CICAD reference dose (TDI – Tolerable Daily Intake). An “x” indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concentration data available	Physicochemical data available	IPCS Chronic TDI <sup>a</sup> (mg/kg-day)
Heptachlor	76-44-8		x	0.0001
Strontium	7440-24-6	x		0.13
Chloroform	67-66-3	x	x	0.015
Mercury	7439-97-6	x		0.002
Barium	7440-39-3	x		0.02
Beryllium	7440-41-7	x		0.002
<i>Ethylene glycol</i>	<i>107-21-1</i>		x	<i>0.05</i>
Tetrachloroethene	127-18-4		x	0.05
<i>Chromium (VI)</i>	<i>18540-29-9</i>			<i>0.0009</i>
Diethyl phthalate	84-66-2		x	5

IPCS = International Programme on Chemical Safety; CICAD = Concise International Chemical Assessment Documents

<sup>a</sup> Tolerable Daily Intake (TDI): An estimate of the intake of a substance, expressed on a body mass basis, to which an individual in a (sub) population may be exposed daily over its lifetime without appreciable health risk.

**Table G-2d. Chemicals reported to be detected in flowback or produced water, with available less-than-chronic RfVs and OSFs.**

Chemicals are ranked by PPRTV subchronic reference dose (sRfD). The "--" symbol indicates that no value was available from the sources consulted. Additionally, an "x" indicates the availability of measured concentration data in flowback or produced water (see Appendix E) and physicochemical properties data from EPI Suite™ (see Appendix C). Italicized chemicals are found in both fracturing fluids and flowback/produced water.

Chemical name	CASRN	Concentration data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD <sup>a</sup> (mg/kg-day)	Acute oral MRL <sup>b</sup> (mg/kg-day)	Intermediate oral MRL <sup>c</sup> (mg/kg-day)
Aldrin	309-00-2		x	0.00004	0.002	--
Antimony	7440-36-0	x		0.0004	--	--
Vanadium	7440-62-2	x		0.0007	--	0.01
Lithium	7439-93-2	x		0.002	--	--
Cobalt	7440-48-4	x		0.003	--	0.01
2-Methylnaphthalene	91-57-6	x	x	0.004	--	--
Methyl bromide	74-83-9		x	0.005	--	0.003
Bromodichloromethane	75-27-4		x	0.008	0.04	--
1,2,3-Trichlorobenzene	87-61-6		x	0.008	--	--
<i>Benzene</i>	<i>71-43-2</i>	x	x	<i>0.01</i>	--	--
p-Cresol	106-44-5	x	x	0.02	--	--
Bromoform	75-25-2		x	0.03	0.7	0.2
<i>Ethylbenzene</i>	<i>100-41-4</i>	x	x	<i>0.05</i>	--	<i>0.4</i>
2,4-Dimethylphenol	105-67-9	x	x	0.05	--	--
Chlorodibromomethane	124-48-1		x	0.07	0.1	--
1,2,4-Trichlorobenzene	120-82-1		x	0.09	--	0.1
Butylbenzene	104-51-8		x	0.1	--	--
Benzyl alcohol	100-51-6	x	x	0.3	--	--
Pyrene	129-00-0	x	x	0.3	--	--
<i>Xylenes</i>	<i>1330-20-7</i>	x	x	<i>0.4</i>	<i>1</i>	<i>0.4</i>
<i>Iron</i>	<i>7439-89-6</i>	x		<i>0.7</i>	--	--
<i>Toluene</i>	<i>108-88-3</i>	x	x	<i>0.8</i>	<i>0.8</i>	<i>0.02</i>
<i>Formic acid</i>	<i>64-18-6</i>		x	<i>0.9</i>	--	--
<i>1,2-Propylene glycol</i>	<i>57-55-6</i>		x	<i>20</i>	--	--

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Chemical name	CASRN	Concentration data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD <sup>a</sup> (mg/kg-day)	Acute oral MRL <sup>b</sup> (mg/kg-day)	Intermediate oral MRL <sup>c</sup> (mg/kg-day)
Acrolein	107-02-8		x	--	--	0.004
1,4-Dioxane	123-91-1	x	x	--	5	0.5
Ethylene glycol	107-21-1		x	--	0.8	0.8
Di(2-ethylhexyl) phthalate	117-81-7	x	x	--	--	0.1
Naphthalene	91-20-3	x	x	--	0.6	0.6
Phenol	108-95-2	x	x	--	1	--
Acetone	67-64-1	x	x	--	--	2
Arsenic	7440-38-2	x		--	0.005	--
Chromium (VI)	18540-29-9			--	--	0.005
Copper	7440-50-8	x		--	0.01	0.01
Zinc	7440-66-6	x		--	--	0.3
Aluminum	7429-90-5	x		--	--	1
Acrylonitrile	107-13-1		x	--	0.1	0.01
Dioctyl phthalate	117-84-0	x	x	--	3	0.4
Tetrachloroethylene	127-18-4		x	--	0.008	0.008
Fluoranthene	206-44-0	x	x	0.1	--	0.4
beta-Hexachlorocyclohexane	319-85-7		x	--	0.05	0.0006
Lindane	58-89-9		x	--	0.003	0.00001
Dieldrin	60-57-1		x	--	--	0.0001
Chloroform	67-66-3	x	x	--	0.3	0.1
Strontium	7440-24-6	x		--	--	2
Tin	7440-31-5	x		--	--	0.3
Barium	7440-39-3	x		--	--	0.2
Boron	7440-42-8	x		--	0.2	0.2
Cadmium	7440-43-9	x		--	--	0.0005
Carbon disulfide	75-15-0	x	x	--	0.01	--
Heptachlor	76-44-8		x	--	0.0006	0.0001
Phosphorus	7723-14-0	x		--	--	0.0002

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Chemical name	CASRN	Concentration data available	Physico-chemical data available	PPRTV	ATSDR	
				sRfD <sup>a</sup> (mg/kg-day)	Acute oral MRL <sup>b</sup> (mg/kg-day)	Intermediate oral MRL <sup>c</sup> (mg/kg-day)
Diethyl phthalate	84-66-2		x	--	7	6
Dibutyl phthalate	84-74-2	x	x	--	0.5	--
Fluorene	86-73-7	x	x	--	--	0.4
<i>Dichloromethane</i>	<i>75-09-2</i>		x	--	<i>0.2</i>	--

<sup>a</sup> Reference dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It can be derived from a no observed-adverse-effect level (NOAEL), lowest observed-adverse-effect level (LOAEL), or benchmark dose (BMD), with uncertainty factors generally applied to reflect limitations of the data used. The RfD is generally used in the EPA's noncancer health assessments. Subchronic RfD (sRfD): Duration of exposure is up to 10% of an average lifespan.

<sup>b</sup> Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Acute MRL: Duration of exposure is 1 to 14 days.

<sup>c</sup> Minimum risk level (MRL): An ATSDR estimate of daily human exposure to a hazardous substance at or below which the substance is unlikely to pose a measurable risk of harmful (adverse), noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a specified time period (acute, intermediate, or chronic). MRLs should not be used as predictors of harmful (adverse) health effects. Intermediate MRL: Duration of exposure is >14 to 364 days.

## G.4. References for Appendix G

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<http://www2.epa.gov/hfstudy/analysis-hydraulic-fracturing-fluid-data-fracfocus-chemical-disclosure-registry-1-pdf>
- [U.S. EPA](#) (U.S. Environmental Protection Agency). (2015e). Human health benchmarks for pesticides. Available online at <http://iaspub.epa.gov/apex/pesticides/f?p=HHBP:HOME>
- [WHO](#) (World Health Organization). (2015). Concise international chemical assessment documents. Available online at <http://www.who.int/ipcs/publications/cicad/en/>

## Appendix H

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# Description of EPA Hydraulic Fracturing Study Publications Cited in This Assessment

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## Appendix H. Description of EPA Hydraulic Fracturing Study Publications Cited in This Assessment

**Table H-1. Titles, descriptions, and citations for EPA hydraulic fracturing study publications cited in this assessment.**

Research project	Description	Citations
<b><i>Analysis of existing data</i></b>		
Literature Review	Review and assessment of existing papers and reports, focusing on peer-reviewed literature	Literature review is incorporated into this document.
Spills Database Analysis	Characterization of hydraulic fracturing-related spills using information obtained from selected state and industry data sources	U.S. EPA (U.S. Environmental Protection Agency). (2015). Review of state and industry spill data: characterization of hydraulic fracturing-related spills [EPA Report]. (EPA/601/R-14/001). Washington, D.C.: Office of Research and Development, U.S. Environmental Protection Agency.
Service Company Analysis	Analysis of information provided by nine hydraulic fracturing service companies in response to a September 2010 information request on hydraulic fracturing operations	Analysis of data received is incorporated into this document. <sup>1</sup>
Well File Review	Analysis of information provided by nine oil and gas operators in response to an August 2011 information request for 350 well files	U.S. EPA (U.S. Environmental Protection Agency). (2015). Review of well operator files for hydraulically fractured oil and gas production wells: Well design and construction [EPA Report]. (EPA/601/R-14/002). Washington, D.C.: Office of Research and Development, U.S. Environmental Protection Agency.  Analysis of data received is also incorporated into this document. <sup>2</sup>

<sup>1</sup> Data received and incorporated into this document is cited as: U.S. EPA (U.S. Environmental Protection Agency). (2013). Data received from oil and gas exploration and production companies, including hydraulic fracturing service companies 2011 to 2013. Non-confidential business information source documents are located in Federal Docket ID: EPA-HQ-ORD2010-0674. Available at <http://www.regulations.gov>

<sup>2</sup> Data received and incorporated into this document is cited as: U.S. EPA (U.S. Environmental Protection Agency). (2011). Sampling data for flowback and produced water provided to EPA by nine oil and gas well operators (non-confidential business information). US Environmental Protection Agency. <http://www.regulations.gov/#!docketDetail:rpp=100:so=DESC:sb=docId:po=0:D=EPA-HQ-ORD-2010-0674>

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Research project	Description	Citations
FracFocus Analysis	Analysis of data compiled from FracFocus 1.0, the national hydraulic fracturing chemical registry operated by the Ground Water Protection Council and the Interstate Oil and Gas Compact Commission	<p>U.S. EPA (U.S. Environmental Protection Agency). (2015). Analysis of hydraulic fracturing fluid data from the FracFocus chemical disclosure registry 1.0 [EPA Report]. (EPA/601/R-14/003). Washington, D.C.: Office of Research and Development, U.S. Environmental Protection Agency. <a href="http://www2.epa.gov/hfstudy/analysis-hydraulic-fracturing-fluid-data-fracfocus-chemical-disclosure-registry-1-pdf">http://www2.epa.gov/hfstudy/analysis-hydraulic-fracturing-fluid-data-fracfocus-chemical-disclosure-registry-1-pdf</a></p> <p>U.S. EPA (U.S. Environmental Protection Agency). (2015). Analysis of hydraulic fracturing fluid data from the FracFocus chemical disclosure registry 1.0: project database. Washington, D.C.: U.S. Environmental Protection Agency, Office of Research and Development.</p> <p>U.S. EPA (U.S. Environmental Protection Agency). (2015). Analysis of hydraulic fracturing fluid data from the FracFocus chemical disclosure registry 1.0: Data management and quality assessment report [EPA Report]. (EPA/601/R-14/006). Washington, D.C.: U.S. Environmental Protection Agency, Office of Research and Development. <a href="http://www2.epa.gov/sites/production/files/2015-03/documents/fracfocus_data_management_report_final_032015_508.pdf">http://www2.epa.gov/sites/production/files/2015-03/documents/fracfocus_data_management_report_final_032015_508.pdf</a></p>

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Research project	Description	Citations
<b>Scenario evaluations</b>		
Subsurface Migration Modeling	Numerical modeling of subsurface fluid migration scenarios that explore the potential for fluids, including liquids and gases to move from the fractured zone to drinking water aquifers	<p>Kim, J; Moridis, GJ. (2013). Development of the T+M coupled flow–geomechanical simulator to describe fracture propagation and coupled flow–thermal–geomechanical processes in tight/shale gas systems. <i>Computers and Geosciences</i> 60: 184-198. <a href="http://dx.doi.org/10.1016/j.cageo.2013.04.023">http://dx.doi.org/10.1016/j.cageo.2013.04.023</a></p> <p>Kim, J; Moridis, GJ. (In Press). Numerical analysis of fracture propagation during hydraulic fracturing operations in shale gas systems. <i>International Journal of Rock Mechanics and Mining Sciences</i>.</p> <p>Kim, J; Um, ES; Moridis, GJ. (2014). Fracture Propagation, Fluid Flow, and Geomechanics of Water-Based Hydraulic Fracturing in Shale Gas Systems and Electromagnetic Geophysical Monitoring of Fluid Migration. SPE Hydraulic Fracturing Technology Conference, The Woodlands, Texas, USA. <a href="http://dx.doi.org/10.2118/168578-MS">http://dx.doi.org/10.2118/168578-MS</a></p> <p>Reagan, MT; Moridis, GJ; Johnson, JN; Keen, ND. (2015). Numerical simulation of the environmental impact of hydraulic fracturing of tight/shale gas reservoirs on near-surface groundwater: background, base cases, shallow reservoirs, short-term gas and water transport. <i>Water Resour Res</i> 51: 1-31. <a href="http://dx.doi.org/10.1002/2014WR016086">http://dx.doi.org/10.1002/2014WR016086</a></p> <p>Rutqvist, J; Rinaldi, AP; Cappa, F; Moridis, GJ. (2013). Modeling of fault reactivation and induced seismicity during hydraulic fracturing of shale-gas reservoirs. <i>Journal of Petroleum Science and Engineering</i> 107: 31-44. <a href="http://dx.doi.org/10.1016/j.petrol.2013.04.023">http://dx.doi.org/10.1016/j.petrol.2013.04.023</a></p> <p>Rutqvist, J; Rinaldi, AP; Cappa, F; Moridis, GJ. (2015). Modeling of fault activation and seismicity by injection directly into a fault zone associated with hydraulic fracturing of shale-gas reservoirs. <i>Journal of Petroleum Science and Engineering</i> 127: 377-386. <a href="http://dx.doi.org/10.1016/j.petrol.2015.01.019">http://dx.doi.org/10.1016/j.petrol.2015.01.019</a></p>
Surface Water Modeling	Modeling of concentrations of selected chemicals at public water supplies downstream from wastewater treatment facilities that discharge treated hydraulic fracturing wastewater to surface waters	Weaver, JW; Xu, J; Mravik, SC. (In Press) Scenario analysis of the impact on drinking water intakes from bromide in the discharge of treated oil and gas waste water. <i>J Environ Eng</i> .

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Research project	Description	Citations
Water Availability Modeling	Assessment and modeling of current and future scenarios exploring the impact of water usage for hydraulic fracturing on drinking water availability in the Upper Colorado River Basin and the Susquehanna River Basin	U.S. EPA (U.S. Environmental Protection Agency). (2015). Case study analysis of the impacts of water acquisition for hydraulic fracturing on local water availability [EPA Report]. (EPA/600/R-14/179). Washington, D.C.
<b>Laboratory studies</b>		
Source Apportionment Studies	Identification and quantification of the source(s) of high bromide and chloride concentrations at public water supply intakes downstream from wastewater treatment plants discharging treated hydraulic fracturing wastewater to surface waters	U.S. EPA (U.S. Environmental Protection Agency). (2015). Sources contributing bromide and inorganic species to drinking water intakes on the Allegheny river in western Pennsylvania [EPA Report]. (EPA/600/R-14/430). Washington, D.C.
Analytical Method Development	Development of analytical methods for selected chemicals found in hydraulic fracturing fluids or wastewater	DeArmond, PD; DiGoregorio, AL. (2013). Characterization of liquid chromatography-tandem mass spectrometry method for the determination of acrylamide in complex environmental samples. Anal Bioanal Chem 405: 4159-4166. <a href="http://dx.doi.org/10.1007/s00216-013-6822-4">http://dx.doi.org/10.1007/s00216-013-6822-4</a> DeArmond, PD; DiGoregorio, AL. (2013). Rapid liquid chromatography-tandem mass spectrometry-based method for the analysis of alcohol ethoxylates and alkylphenol ethoxylates in environmental samples. J Chromatogr A 1305: 154-163. <a href="http://dx.doi.org/10.1016/j.chroma.2013.07.017">http://dx.doi.org/10.1016/j.chroma.2013.07.017</a>

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Research project	Description	Citations
Analytical Method Development (cont.)	Development of analytical methods for selected chemicals found in hydraulic fracturing fluids or wastewater (cont.)	U.S. EPA (U.S. Environmental Protection Agency). (2014). Development of rapid radiochemical method for gross alpha and gross beta activity concentration in flowback and produced waters from hydraulic fracturing operations [EPA Report]. (EPA/600/R-14/107). Washington, D.C. <a href="http://www2.epa.gov/hfstudy/development-rapid-radiochemical-method-gross-alpha-and-gross-beta-activity-concentration">http://www2.epa.gov/hfstudy/development-rapid-radiochemical-method-gross-alpha-and-gross-beta-activity-concentration</a> U.S. EPA (U.S. Environmental Protection Agency). (2014). The verification of a method for detecting and quantifying diethylene glycol, triethylene glycol, tetraethylene glycol, 2-butoxyethanol and 2-methoxyethanol in ground and surface waters [EPA Report]. (EPA/600/R-14/008). Washington, D.C. <a href="http://www2.epa.gov/hfstudy/verification-method-detecting-and-quantifying-diethylene-glycol-triethylene-glycol">http://www2.epa.gov/hfstudy/verification-method-detecting-and-quantifying-diethylene-glycol-triethylene-glycol</a>
<b>Retrospective case studies</b>		
<i>Investigations of whether reported drinking water impacts may be associated with or caused by hydraulic fracturing activities</i>		
Las Animas and Huerfano Counties, Colorado	Investigation of potential drinking water impacts from coalbed methane extraction in the Raton Basin	U.S. EPA (U.S. Environmental Protection Agency). (2015). Retrospective case study in the Raton Basin, Colorado: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/091). Washington, D.C.
Dunn County, North Dakota	Investigation of potential drinking water impacts from a well blowout during hydraulic fracturing for oil in the Bakken Shale	U.S. EPA (U.S. Environmental Protection Agency). (2015). Retrospective case study in Killdeer, North Dakota: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/103). Washington, D.C.
Bradford County, Pennsylvania	Investigation of potential drinking water impacts from shale gas development in the Marcellus Shale	U.S. EPA (U.S. Environmental Protection Agency). (2014). Retrospective case study in northeastern Pennsylvania: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/088). Washington, D.C.
Washington County, Pennsylvania	Investigation of potential drinking water impacts from shale gas development in the Marcellus Shale	U.S. EPA (U.S. Environmental Protection Agency). (2015). Retrospective case study in southwestern Pennsylvania: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/084). Washington, D.C.

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<b>Research project</b>	<b>Description</b>	<b>Citations</b>
Wise County, Texas	Investigation of potential drinking water impacts from shale gas development in the Barnett Shale	U.S. EPA (U.S. Environmental Protection Agency). (2015). Retrospective case study in Wise County, Texas: study of the potential impacts of hydraulic fracturing on drinking water resources [EPA Report]. (EPA 600/R-14/090). Washington, D.C.

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# Appendix I

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## Unit Conversions

## Appendix I. Unit Conversions

### 1 LENGTH

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2 1 in (inch) = 2.54 cm (centimeters)  
 3 25.4 mm (millimeters)  
 4 25,400  $\mu\text{m}$  (microns)

5 1 ft (foot) = 0.3048 m (meters)  
 6 30.48 cm

7 1 mi (mile) = 5,280 ft  
 8 1,609.344 m  
 9 1.6093 km (kilometers)

### 10 AREA

---

11 1 ft<sup>2</sup> (square foot) = 0.0929 m<sup>2</sup> (square meters)

12 1 acre = 43,560 ft<sup>2</sup>  
 13 = 0.0016 mi<sup>2</sup> (square miles)  
 14 = 0.4047 ha (hectares)  
 15 = 4,046.825 m<sup>2</sup>

16 1 mi<sup>2</sup> = 639.9974 ac  
 17 = 258.9988 ha  
 18 = 2.5899 km<sup>2</sup> (square kilometers)

### 19 MASS

---

20 1 lb (pound) = 453.5924 g (grams)  
 21 = 0.4536 kg (kilograms)

22 1 ton (short ton, U.S.) = 2,000 lbs  
 23 = 907.185 kg  
 24 = 0.9072 metric tons

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**1 VOLUME OR CAPACITY (LIQUID MEASURE)**


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2	1 bbl (barrel)	=	42 gal (gallons, U.S.)
3		=	158.9873 L (liters)
4	1 gal	=	231 in <sup>3</sup> (cubic inches)
5		=	0.1337 ft <sup>3</sup> (cubic feet)
6		=	3.7854 L
7		=	0.0039 m <sup>3</sup> (cubic meters)
8		=	3.7854 × 10 <sup>-9</sup> Mm <sup>3</sup> (million cubic meters)
9	1 Mgal (million gallons)	=	1.3368 × 10 <sup>5</sup> ft <sup>3</sup>
10	1 ft <sup>3</sup>	=	1,728 in <sup>3</sup>
11		=	7.4805 gal
12		=	28.3169 L
13		=	0.0283 m <sup>3</sup>
14	1 mi <sup>3</sup> (cubic mile)	=	4.1682 km <sup>3</sup> (cubic kilometers)
15			

**16 CONCENTRATION**


---

17	1 mg/L (milligram per liter)	=	1.0 × 10 <sup>-6</sup> kg/L (kilograms per liter)
18		=	1.0 × 10 <sup>-3</sup> g/L (grams per liter)
19		=	1,000 µg/L (micrograms per liter)
20		=	1.001 ppm (parts per million)
21		=	8.3454 × 10 <sup>-6</sup> lb/gal (pounds per gallon)
22		=	6.2428 × 10 <sup>-5</sup> lb/ft <sup>3</sup> (pounds per cubic foot)

**23 SPEED**


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24	1 mi/hr (mile per hour)	=	1.4666̄ ft/s (feet per second)
25		=	0.4470 m/s (meters per second)

**26 DENSITY**


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27	1 g/mL	=	1,000 g/L
28		=	1.0 × 10 <sup>6</sup> mg/L

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**1 VOLUME PER UNIT TIME**


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2	1 ft <sup>3</sup> /s (cubic foot per second)	=	448.8312 gpm (gallons per minute)
3		=	0.6163 Mgal/d (million gallons per day)
4		=	28.3169 L/s (liters per second)
5		=	0.0283 m <sup>3</sup> /s (cubic meters per second)
6	1 ft <sup>3</sup> /day (cubic feet per day)	=	0.0052 gpm
7		=	7.4805 gpd
8		=	0.0283 m <sup>3</sup> /d (cubic meters per day)
9			
10	1 bbl/day (barrel per day)	=	42 gpd
11		=	158.9873 L/d (liters per day)

**12 PRESSURE**


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13	1 psi (pound per square inch)	=	6,894.7573 Pa (pascals)
14		=	0.068 atm (standard atmospheres)

**15 RADIATION**


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**16 Activity**

17	1 Ci (curie)	=	$3.7 \times 10^{10}$ decays per second
18	1 Bq (becquerel)	≈	$2.703 \times 10^{-11}$ Ci
19		≈	27.027 pCi (picocuries)
20	1 pCi	=	0.037 Bq
21		=	0.037 decays per second
22		=	2.22 decays per minute

**23 Exposure**

24	1 rem (röntgen equivalent in man)	=	0.01 Sv (sieverts)
25	1 Sv	=	1 J/kg (joule per kilogram)

**26 ELECTRIC CONDUCTANCE**


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27	1 S (siemen)	=	1 Ω <sup>-1</sup> (reciprocal of resistance)
28		=	1 A/V (ampere per volt)
29		=	1 kg <sup>-1</sup> • m <sup>-2</sup> • s <sup>3</sup> • A <sup>2</sup> (second cubed- ampere squared per kilogram-square meter)
30			
31		=	1.0 × 10 <sup>6</sup> μS (microsiemens)

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**1 TEMPERATURE**

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2  $[\text{°F (degrees, Fahrenheit)} - 32] \times 5/9 = \text{°C (degrees, Celsius)}$

**3 PERMEABILITY**

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4  $1 \text{ cm}^2 = 1.0 \times 10^{-4} \text{ m}^2$   
5  $\approx 1.0 \times 10^8 \text{ D (darcys)}$   
6  $1 \text{ D} \approx 1.0 \times 10^{-12} \text{ m}^2$   
7  $= 1,000 \text{ mD (millidarcys)}$   
8  $= 1.0 \times 10^6 \text{ }\mu\text{D (microdarcys)}$

## Appendix J

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### Glossary

## Appendix J. Glossary

### J.1. Glossary Terms and Definitions

- 1 **Acid mine drainage:** Flow of water from areas that have been mined for coal or other mineral ores.  
2 The water has a low pH because of its contact with sulfur-bearing material and is harmful to  
3 aquatic organisms. ([U.S. EPA, 2013d](#))
- 4 **Additive:** A single chemical or chemical mixture designed to serve a specific purpose in the  
5 hydraulic fracturing fluid.<sup>1</sup>
- 6 **Adsorption:** Adhesion of molecules of gas, liquid, or dissolved solids to a surface. ([U.S. EPA, 2013d](#))
- 7 **Advection:** A mechanism for moving chemicals in flowing water, where a chemical moves along  
8 with the flow of the water itself.
- 9 **Aeration:** A process that promotes biological degradation of organic matter in water. The process  
10 may be passive (as when waste is exposed to air) or active (as when a mixing or bubbling device  
11 introduces the air). ([U.S. EPA, 2013d](#))
- 12 **Aerobic mesophiles:** Microorganisms that use oxygen for energy production and are tolerant of  
13 moderate temperatures.
- 14 **Analyte:** The element, ion, or compound that an analysis seeks to identify; the compound of  
15 interest. ([U.S. EPA, 2013d](#))
- 16 **Annulus:** Refers to either the space between the casing of a well and the wellbore or the space  
17 between any two strings of tubing or casing. ([U.S. EPA, 2013d](#))
- 18 **API number:** A unique identifying number for all oil and gas wells drilled in the United States. The  
19 system was developed by the American Petroleum Institute. ([Oil and Gas Mineral Services, 2010](#))
- 20 **Aquifer:** An underground geological formation, or group of formations, containing water. A source  
21 of ground water for wells and springs. ([U.S. EPA, 2013d](#))
- 22 **Base fluid:** The fluid into which additives and proppants are mixed to formulate a hydraulic  
23 fracturing fluid.
- 24 **Basin:** A depression in the crust of the earth, caused by plate tectonic activity and subsidence, in  
25 which sediments accumulate. Sedimentary basins vary from bowl-shaped to elongated troughs.  
26 Basins can be bounded by faults. Rift basins are commonly symmetrical; basins along continental  
27 margins tend to be asymmetrical. If rich hydrocarbon source rocks occur in combination with  
28 appropriate depth and duration of burial, then a petroleum system can develop within the basin.

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<sup>1</sup> Definitions that have no associated citation in this glossary were developed for this assessment.

- 1 Most basins contain some amount of shale, thus providing opportunities for shale gas exploration  
2 and production. ([Schlumberger, 2014](#))
- 3 **Biogenic:** Methane that is produced in shallower formations by bacterial activity in anaerobic  
4 conditions. It is the ultimate dissimilation product of microbially mediated reactions of organic  
5 molecules.
- 6 **Blowout preventer (BOP):** Casinghead equipment that prevents the uncontrolled flow of oil, gas,  
7 and mud from the well by closing around the drill pipe or sealing the hole. ([Oil and Gas Mineral  
8 Services, 2010](#))
- 9 **Brackish water:** Mixed fresh and salt waters. Used here to qualitatively refer to water that contains  
10 higher total dissolved solids (TDS) than that typically used for fresh drinking water.
- 11 **BTEX:** An acronym for benzene, toluene, ethylbenzene, and xylenes. These chemicals are a group of  
12 single ringed aromatic hydrocarbon based on the benzene structure. These compounds are found in  
13 petroleum and are of specific importance because of their health effects.
- 14 **Caliper log:** A log that is used to check for any wellbore irregularities. It is run prior to primary  
15 cementing as a means of calculating the amount of cement needed. Also run in conjunction with  
16 other open hole logs for log corrections or run on cased holes to evaluate metal loss. ([NYSDEC,  
17 2011](#))
- 18 **Capillarity:** The action by which the surface of a liquid where it is in contact with a solid is elevated  
19 or depressed depending on the relative attraction of the molecules of the liquid for each other and  
20 for those of the solid. Capillary forces arise from the differential attraction between immiscible  
21 fluids and solid surfaces; these are the forces responsible for capillary rise in small-diameter tubes  
22 and porous materials. ([Adapted from Dake, 1978](#))
- 23 **Casing:** Steel pipe that is lowered into a wellbore. Casing extends from the bottom of the hole to the  
24 surface. ([Schlumberger, 2014](#))
- 25 **Casing inspection logs:** An in situ record of casing thickness and integrity, to determine whether  
26 and to what extent the casing has undergone corrosion. The term refers to an individual  
27 measurement, or a combination of measurements using acoustic, electrical, and mechanical  
28 techniques, to evaluate the casing thickness and other parameters. The log is usually presented  
29 with the basic measurements and an estimate of metal loss. It was first introduced in the early  
30 1960s. Today the terms casing-evaluation log and pipe-inspection log are used synonymously.  
31 ([Schlumberger, 2014](#))
- 32 **Cation exchange capacity:** The total amount of cations (positively charged ions) that a soil can  
33 hold.

- 1 **Cement:** Material used to support and seal the well casing to the rock formations exposed in the  
2 borehole. Cement also protects the casing from corrosion and prevents movement of injectate up  
3 the borehole. ([U.S. EPA, 2013d](#))
- 4 **Cement squeeze:** A remedial cementing operation designed to force cement into leak paths in  
5 wellbore tubulars. The required squeeze pressure is achieved by carefully controlling pump  
6 pressure. Squeeze cementing operations may be performed to repair poor primary cement jobs,  
7 isolate perforations, or repair damaged casing or liner. ([Schlumberger, 2014](#))
- 8 **Centralized waste treatment facility (CWT):** any facility that treats (for disposal, recycling or  
9 recovery of material) any hazardous or non-hazardous industrial wastes, hazardous or non-  
10 hazardous industrial wastewater, and/or used material received from off-site. ([U.S. EPA, 2012b](#))
- 11 **Coalbed methane:** Methane contained in coal seams. A coal seam is a layer or stratum of coal  
12 parallel to the rock stratification. ([U.S. EPA, 2013d](#))
- 13 **Collapse pressure:** The pressure at which a tube, or vessel, will catastrophically deform as a result  
14 of differential pressure acting from outside to inside of the vessel or tube. ([Schlumberger, 2014](#))
- 15 **Collar:** A threaded coupling used to join two lengths of pipe such as production tubing, casing, or  
16 liner. The type of thread and style of collar varies with the specifications and manufacturer of the  
17 tubing. ([Schlumberger, 2014](#))
- 18 **Combination truck:** A truck tractor or a truck tractor pulling any number of trailers. ([U.S.](#)  
19 [Department of Transportation, 2012](#))
- 20 **Community water systems:** Public water systems that supply water to the same population year-  
21 round. ([U.S. EPA, 2013c](#))
- 22 **Completion:** A term used to describe the assembly of equipment at the bottom of the well that is  
23 needed to enable production from an oil or gas well. It can also refer to the activities and methods  
24 (including hydraulic fracturing) used to prepare a well for production following drilling.
- 25 **Complexation:** A reaction between two chemicals that form a new complex, either through  
26 covalent bonding or ionic forces. This often results in one chemical solubilizing the other.
- 27 **Compressive strength:** Measure of the ability of a substance to withstand compression. ([NYSDEC,](#)  
28 [2011](#))
- 29 **Conductor casing:** This large diameter casing is usually the first string of casing in a well. It is set  
30 or driven into the unconsolidated material where the well will be drilled to keep the loose material  
31 from caving in. ([NYSDEC, 2011](#))
- 32 **Confidential business information (CBI):** Information that contains trade secrets, commercial or  
33 financial information, or other information that has been claimed as confidential by the submitter.  
34 The EPA has special procedures for handling such information. ([U.S. EPA, 2013d](#))

- 1 **Contaminant:** A substance that is either present in an environment where it does not belong or is  
2 present at levels that might cause harmful (adverse) health effects. ([U.S. EPA, 2013d](#))
- 3 **Conventional reservoir:** A reservoir in which buoyant forces keep hydrocarbons in place below a  
4 sealing caprock. Reservoir and fluid characteristics of conventional reservoirs typically permit oil  
5 or natural gas to flow readily into wellbores. The term is used to make a distinction from shale and  
6 other unconventional reservoirs, in which gas might be distributed throughout the reservoir at the  
7 basin scale, and in which buoyant forces or the influence of a water column on the location of  
8 hydrocarbons within the reservoir are not significant. ([Schlumberger, 2014](#))
- 9 **Crosslinked gels:** linear gels that are linked together by chemicals called crosslinkers, which may  
10 link two or more chains together.
- 11 **Crude oil:** A general term for unrefined petroleum or liquid petroleum. ([Schlumberger, 2014](#))
- 12 **Cumulative effects:** Refers to combined changes in the environment that can take place as a result  
13 of multiple activities over time and/or space.
- 14 **Cumulative water use/cumulative water:** Refers to the amount of water used or consumed by all  
15 hydraulic fracturing wells in a given area per year.
- 16 **Cyclical stress:** Refers to stress caused by frequent or rapid changes in temperature or pressure.
- 17 **Deviated well:** Any non-horizontal well in which the well bottom is intentionally located at a  
18 distance (e.g., hundreds of feet) laterally from the wellhead.
- 19 **Discharge:** Any emission (other than natural seepage), intentional or unintentional. Includes, but is  
20 not limited to, spilling, leaking, pumping, pouring, emitting, emptying, or dumping. ([U.S. EPA,](#)  
21 [2013d](#))
- 22 **Disinfection byproduct (DBP):** A compound formed by the reaction of a disinfectant such as  
23 chlorine with organic material in the water supply. ([U.S. EPA, 2013d](#))
- 24 **Domestic water use:** Includes indoor and outdoor water uses at residences, and includes uses such  
25 as drinking, food preparation, bathing, washing clothes and dishes, flushing toilets, watering lawns  
26 and gardens, and maintaining pools. ([USGS, 2015](#))
- 27 **Drill bit:** The tool used to crush or cut rock. Most bits work by scraping or crushing the rock as part  
28 of a rotational motion, while some bits work by pounding the rock vertically. ([Schlumberger, 2014](#))
- 29 **Drill collar:** A component of a drill string that provides weight on the bit for drilling. Drill collars  
30 are thick-walled tubular pieces machined from solid bars of steel, usually plain carbon steel but  
31 sometimes of nonmagnetic nickel-copper alloy or other nonmagnetic premium alloys.  
32 ([Schlumberger, 2014](#))
- 33 **Drill cuttings:** Ground rock produced by the drilling process.

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- 1 **Drill string:** The combination of the drillpipe, the bottomhole assembly, and any other tools used to  
2 make the drill bit turn at the bottom of the wellbore. ([Schlumberger, 2014](#))
- 3 **Drilling fluid:** Any of a number of liquid and gaseous fluids and mixtures of fluids and solids used  
4 when drilling boreholes. ([Adapted from Schlumberger, 2014](#))
- 5 **Drinking water resource:** Any body of ground water or surface water that now serves, or in the  
6 future could serve, as a source of drinking water for public or private use ([U.S. EPA, 2013d](#))
- 7 **Dry gas:** Refers to natural gas that occurs in the absence of liquid hydrocarbons. ([Adapted from](#)  
8 [Schlumberger, 2014](#))
- 9 **Effluent:** Waste material being discharged into the environment, either treated or untreated. ([U.S.](#)  
10 [EPA, 2013d](#))
- 11 **Facultative anaerobes:** Microorganisms that can use oxygen for energy production if it is present  
12 in their environment, but can also use alternatives for energy production if no oxygen is present.
- 13 **Fault:** A fracture or fracture zone along which there has been displacement of the sides relative to  
14 each other. ([NYSDEC, 2011](#))
- 15 **Field:** Area of oil and gas production with at least one common reservoir for the entire area. ([Oil](#)  
16 [and Gas Mineral Services, 2010](#))
- 17 **Flowback:** The term is defined multiple ways in the literature. In general, it is either fluids  
18 predominantly containing hydraulic fracturing fluid that return from a well to the surface or a  
19 process used to prepare the well for production.
- 20 **Fluid:** A substance that flows when exposed to an external pressure; fluids include both liquids and  
21 gases.
- 22 **Fluid formulation:** The entire suite of chemicals, proppant, and base fluid injected into a well  
23 during hydraulic fracturing. ([U.S. EPA, 2013d](#))
- 24 **Formation:** A body of earth material with distinctive and characteristic properties and a degree of  
25 homogeneity in its physical properties. ([U.S. EPA, 2013d](#))
- 26 **Formation packer:** A specialized casing part that has the same inner diameter as the casing but  
27 whose outer diameter expands to make contact with the formation and seal the annulus between  
28 the casing and formation, preventing migration of fluids.
- 29 **Formation fluid:** Fluid that occurs naturally within the pores of rock. These fluids consist primarily  
30 of water, with varying concentrations of total dissolved solids, but may also contain oil or gas.  
31 Sometimes referred to as native fluids, native brines, or reservoir fluids.
- 32 **FracFocus Registry:** A registry for oil and gas well operators to disclose information about  
33 hydraulic fracturing well locations, and water and chemical use during hydraulic fracturing
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- 1 operations developed by the Ground Water Protection Council and the Interstate Oil and Gas  
2 Compact Commission.
- 3 **Fracture:** A crack or breakage surface within a rock.
- 4 **Fracture geometry:** Refers to characteristics of the fracture such as height and aperture (width).
- 5 **Fresh water:** Qualitatively refers to water with relatively low TDS that is most readily available for  
6 drinking water currently.
- 7 **Gelled fluids:** Fracturing fluids that are usually water-based with added gels to increase the fluid  
8 viscosity to aid in the transport of proppants. ([Spellman, 2012](#); [Gupta and Valkó, 2007](#))
- 9 **Ground water:** In the broadest sense, all subsurface water; more commonly that part of the  
10 subsurface water in the saturated zone. ([Solley et al., 1998](#))
- 11 **Halite:** A soft, soluble evaporate mineral commonly known as salt or rock salt. Can be critical in  
12 forming hydrocarbon traps and seals because it tends to flow rather than fracture during  
13 deformation, thus preventing hydrocarbons from leaking out of a trap even during and after some  
14 types of deformation. ([Schlumberger, 2014](#))
- 15 **Hazard evaluation:** A component of risk assessment that involves gathering and evaluating data  
16 on the types of health injuries or diseases (e.g., cancer) that may be produced by a chemical and on  
17 the conditions of exposure under which such health effects are produced.
- 18 **Hazard identification:** A process for determining if a chemical or a microbe can cause adverse  
19 health effects in humans and what those effects might be. ([U.S. EPA, 2013d](#))
- 20 **Henry's law constant:** Ratio of a chemical's vapor pressure in the atmosphere to its solubility in  
21 water. The higher the Henry's law constant, the more volatile the compound will be from water.  
22 ([NYSDEC, 2011](#))
- 23 **Horizontal drilling:** Drilling a portion of a well horizontally to expose more of the formation  
24 surface area to the wellbore. ([Oil and Gas Mineral Services, 2010](#))
- 25 **Horizontal well:** A well that is drilled vertically up to a point known as the kickoff point, where the  
26 well turns toward the horizontal, extending into and parallel with the approximately horizontal  
27 targeted producing formation.
- 28 **Hydraulic fracturing:** A stimulation technique used to increase production of oil and gas.  
29 Hydraulic fracturing involves the injection of fluids under pressures great enough to fracture the  
30 oil- and gas-production formations. ([U.S. EPA, 2011a](#))
- 31 **Hydraulic fracturing fluids:** Engineered fluids, typically consisting of a base fluid, additives, and  
32 proppant, that are pumped under high pressure into the well to create and hold open fractures in  
33 the formation.

- 1 **Hydraulic fracturing wastewater:** Flowback and produced water that is managed using practices  
2 that include but are not limited to reuse in subsequent hydraulic fracturing operations, treatment  
3 and discharge, and injection into disposal wells.
- 4 **Hydraulic fracturing water cycle:** The cycle of water in the hydraulic fracturing process,  
5 encompassing the acquisition of water, chemical mixing of the fracturing fluid, injection of the fluid  
6 into the formation, the production and management of flowback and produced water, and the  
7 ultimate treatment and disposal of hydraulic fracturing wastewaters.
- 8 **Hydraulic gradient:** Slope of a water table or potentiometric surface. More specifically, change in  
9 the hydraulic head per unit of distance in the direction of the maximum rate of decrease. ([U.S. EPA,](#)  
10 [2013d](#))
- 11 **Hydrocarbon:** An organic compound containing only hydrogen and carbon, often occurring in  
12 petroleum, natural gas, and coal. ([U.S. EPA, 2013d](#))
- 13 **Hydrostatic pressure:** The pressure exerted by a column of fluid at a given depth.
- 14 **Imbibition:** The displacement of a non-wet fluid (i.e., gas) by a wet fluid (typically water). ([Adapted](#)  
15 [from Dake, 1978](#))
- 16 **Immiscible:** The chemical property in which two or more liquids or phases are incapable of  
17 attaining homogeneity. ([U.S. EPA, 2013d](#))
- 18 **Impact:** Any observed change in the quality or quantity of drinking water resources, regardless of  
19 severity, that results from a mechanism.
- 20 **Impact, potential:** Any change in the quality or quantity of drinking water resources that could  
21 logically occur, but has not yet been observed, as the result of a mechanism or potential mechanism.
- 22 **Induced fracture:** A fracture created during hydraulic fracturing.
- 23 **Injection well:** A well into which fluids are being injected (40 CFR 144.3).
- 24 **Integrated risk information system (IRIS):** An electronic database that contains the EPA's latest  
25 descriptive and quantitative regulatory information about chemical constituents. Files on chemicals  
26 maintained in IRIS contain information related to both noncarcinogenic and carcinogenic health  
27 effects. ([U.S. EPA, 2013d](#))
- 28 **Intermediate casing:** Casing that seals off intermediate depths and geologic formations that may  
29 have considerably different reservoir pressures than deeper zones to be drilled. ([Devereux, 1998;](#)  
30 [Baker, 1979](#))
- 31 **Karst:** A type of topography that results from dissolution and collapse of carbonate rocks, such as  
32 limestone, dolomite, and gypsum, and that is characterized by closed depressions or sinkholes,  
33 caves, and underground drainage. ([Solley et al., 1998](#))

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- 1 **Kill fluid:** A weighted fluid with a density that is sufficient to overcome the formation pressure and  
2 prevent fluids from flowing up the wellbore.
- 3 **Large truck:** A truck with a gross vehicle weight rating greater than 10,000 pounds. ([U.S.](#)  
4 [Department of Transportation, 2012](#))
- 5 **Lateral:** A horizontal section of a well.
- 6 **Leakoff:** The fraction of the injected fluid that infiltrates into the formation (e.g., through an  
7 existing natural fissure) and is not recovered during production.
- 8 **Linear gel:** a series of chemicals linked together so that they form a chain.
- 9 **Liner:** A casing string that does not extend to the top of the wellbore, but instead is anchored or  
10 suspended from inside the bottom of the previous casing string. ([Schlumberger, 2014](#))
- 11 **Lost cement:** Refers to a failure of the cement to be circulated back to the surface, indicating that  
12 the cement has escaped into the formation.
- 13 **Lowest-observable-adverse effect level (LOAEL):** The lowest exposure level at which there are  
14 biologically significant increases in frequency or severity of adverse effects between the exposed  
15 population and its appropriate control group.
- 16 **Maximum allowable daily level (MADL):** The maximum allowable daily level of a reproductive  
17 toxicant at which the chemical would have no observable adverse reproductive effect, assuming  
18 exposure at 1,000 times that level.
- 19 **Maximum contaminant level (MCL):** The highest level of a contaminant that is allowed in  
20 drinking water. MCLs are enforceable standards. ([U.S. EPA, 2014b](#))
- 21 **Mechanical integrity:** The absence of significant leakage within the injection tubing, casing, or  
22 packer (known as internal mechanical integrity), or outside of the casing (known as external  
23 mechanical integrity). ([U.S. EPA, 2013d](#))
- 24 **Mechanism:** A means or series of events by which an activity within the hydraulic fracturing water  
25 cycle has been observed to change the quality or quantity of drinking water resources.
- 26 **Mechanism, potential:** A means or series of events by which hydraulic fracturing activities could  
27 logically or theoretically (for instance, based on modeling) change the quality or quantity of  
28 drinking water resources but one that has not yet been observed.
- 29 **Mechanism, suspected:** A means or series of events by which hydraulic fracturing activities could  
30 logically have resulted in an observed change in the quality or quantity of drinking water resources.  
31 Available evidence may or may not be sufficient to determine if it is the *only* mechanism that caused  
32 the observed change.

- 1 **Metropolitan combined statistical area:** A core urban area of 50,000 or more people. ([U.S.](#)  
2 [Census Bureau, 2013](#))
- 3 **Microaerophiles:** Microorganisms that require small amounts of oxygen for energy production.
- 4 **Microannuli:** Very small channels that form in the cement and that may serve as pathways for fluid  
5 migration to drinking water resources.
- 6 **Micropolitan combined statistical area:** An urban core of at least 10,000, but less than 50,000,  
7 people. ([U.S. Census Bureau, 2013](#))
- 8 **Microseismic monitoring:** A technique to track the propagation of a hydraulic fracture as it  
9 advances through a formation. ([Schlumberger, 2014](#))
- 10 **Minimum risk level (MRL):** An estimate of daily human exposure to a hazardous substance at or  
11 below which the substance is unlikely to pose a measurable risk of harmful (adverse),  
12 noncancerous effects. MRLs are calculated for a route of exposure (inhalation or oral) over a  
13 specified time period (acute, intermediate, or chronic).
- 14 **Mobility:** The ratio of effective permeability to phase viscosity. The overall mobility is a sum of the  
15 individual phase viscosities. Well productivity is directly proportional to the product of the mobility  
16 and the layer thickness product. ([Schlumberger, 2014](#))
- 17 **National Pollution Discharge Elimination System (NPDES):** A national program under  
18 Section 402 of the Clean Water Act for regulation of discharges of pollutants from point sources to  
19 waters of the United States. Discharges are illegal unless authorized by an NPDES permit. ([U.S. EPA,](#)  
20 [2013d](#))
- 21 **National Secondary Drinking Water Regulations (NSDWR):** Non-enforceable guidelines  
22 regulating contaminants that may cause cosmetic effects (such as skin or tooth discoloration) or  
23 aesthetic effects (such as taste, odor, or color) in drinking water (also referred to as secondary  
24 standards). ([U.S. EPA, 2014b](#))
- 25 **Natural gas:** A naturally occurring mixture of hydrocarbon and nonhydrocarbon gases in porous  
26 formations beneath the earth's surface, often in association with petroleum. The principal  
27 constituent of natural gas is methane. ([Schlumberger, 2014](#))
- 28 **Natural organic matter (NOM):** Complex organic compounds that are formed from decomposing  
29 plant animal and microbial material in soil and water. ([U.S. EPA, 2013d](#))
- 30 **Non-community water systems:** Water systems that supply water to at least 25 of the same  
31 people at least six months per year, but not year-round. ([U.S. EPA, 2013c](#))
- 32 **Octanol-water partition coefficient ( $K_{ow}$ ):** A coefficient representing the ratio of the solubility of a  
33 compound in octanol (a nonpolar solvent) to its solubility in water (a polar solvent). The higher the  
34  $K_{ow}$ , the more nonpolar the compound. Log  $K_{ow}$  is generally used as a relative indicator of the

- 1 tendency of an organic compound to adsorb to soil. Log  $K_{ow}$  values are generally inversely related to  
2 aqueous solubility and directly proportional to molecular weight. ([U.S. EPA, 2013d](#))
- 3 **Offset well:** An existing wellbore close to a proposed well that provides information for planning  
4 the proposed well. ([Schlumberger, 2014](#))
- 5 **Open hole completion:** A well completion that has no casing or liner set across the reservoir  
6 formation, allowing the produced fluids to flow directly into the wellbore. ([Schlumberger, 2014](#))
- 7 **Oral slope factor (OSF):** An upper-bound, approximating a 95% confidence limit, on the increased  
8 cancer risk from a lifetime oral exposure to an agent. This estimate, usually expressed in units of  
9 proportion (of a population) affected per mg/kg day, is generally reserved for use in the low dose  
10 region of the dose response relationship, that is, for exposures corresponding to risks less than 1 in  
11 100.
- 12 **Organic carbon-water partition coefficient ( $K_{oc}$ ):** A coefficient representing the amount of a  
13 compound that is adsorbed to soil to the amount of a compound that is dissolved in water,  
14 normalized to the total organic carbon content of the soil. The higher the  $K_{oc}$ , the more likely a  
15 compound is to adsorb to soils and sediments, and the less likely it is to migrate with water. Along  
16 with log  $K_{ow}$ , log  $K_{oc}$  is used as a relative indicator of the tendency of an organic compound to adsorb  
17 to soil.
- 18 **Orphaned well:** An inactive oil or gas well with no known (or financially solvent) owner.
- 19 **Overburden:** Material of any nature, consolidated or unconsolidated, that overlies a deposit of  
20 useful minerals or ores. ([U.S. EPA, 2013d](#))
- 21 **Packer:** A device that can be run into a wellbore with a smaller initial outside diameter that then  
22 expands externally to seal the wellbore. ([Schlumberger, 2014](#))
- 23 **Pad fluid:** a mixture of base fluid, typically water and additives designed to create, elongate, and  
24 enlarge fractures along the natural channels of the formation when injected under high pressure.
- 25 **Partial cementing:** Cementing a casing string along only a portion of its length.
- 26 **Passby flow:** A prescribed, low-streamflow threshold below which withdrawals are not allowed.  
27 ([U.S. EPA, 2015d](#))
- 28 **Peer review:** A documented critical review of a specific major scientific and/or technical work  
29 product. Peer review is intended to uncover any technical problems or unresolved issues in a  
30 preliminary or draft work product through the use of independent experts. This information is then  
31 used to revise the draft so that the final work product will reflect sound technical information and  
32 analyses. The process of peer review enhances the scientific or technical work product so that the  
33 decision or position taken by the EPA, based on that product, has a sound and credible basis. ([U.S.](#)  
34 [EPA, 2013d](#))

- 1 **Perforation:** The communication tunnel created from the casing or liner into the reservoir  
2 formation through which injected fluids and oil or gas flows. Also refers to the process of creating  
3 communication channels, e.g., via the use of a jet perforating gun.
- 4 **Permeability:** The ability of a material (e.g., rock or soil) to transmit fluid to move through pore  
5 spaces.
- 6 **Persistence:** The length of time a compound stays in the environment, once introduced. A  
7 compound may persist for less than a second or indefinitely.
- 8 **Physicochemical properties:** The inherent physical and chemical properties of a molecule such as  
9 boiling point, density, physical state, molecular weight, vapor pressure, etc. These properties define  
10 how a chemical interacts with its environment. ([U.S. EPA, 2013d](#))
- 11 **Play:** A set of oil or gas accumulations sharing similar geologic, geographic properties, such as  
12 source rock, hydrocarbon type, and migration pathways. ([Oil and Gas Mineral Services, 2010](#))
- 13 **Poisson's ratio:** A ratio of transverse-to-axial (or latitudinal-to-longitudinal) strain; characterizes  
14 how a material is deformed under pressure.
- 15 **Polar molecule:** A molecule with a slightly positive charge at one part of the molecule and a  
16 slightly negative charge on another. The water molecule, H<sub>2</sub>O, is an example of a polar molecule,  
17 where the molecule is slightly positive around the hydrogen atoms and negative around the oxygen  
18 atom.
- 19 **Porosity:** A measure of pore space, or the percentage of the material (e.g., rock or soil) volume that  
20 can be occupied by oil, gas, or water.
- 21 **Produced water:** Water that flows from oil and gas wells.
- 22 **Production casing:** The deepest casing set and serves primarily as the conduit for producing fluids,  
23 although when cemented to the wellbore, this casing can also serve to seal off other subsurface  
24 zones including ground water resources. ([Devereux, 1998](#); [Baker, 1979](#))
- 25 **Production well:** A well that is used to bring fluids (such as oil or gas) to the surface.
- 26 **Production zone:** Refers to the portion of a subsurface rock zone that contains oil or gas to be  
27 extracted (sometimes using hydraulic fracturing). The production zone is sometimes referred to as  
28 the target zone.
- 29 **Proppant/propping agent:** A granular substance (sand grains, aluminum pellets, or other  
30 material) that is carried in suspension by the fracturing fluid and that serves to keep the cracks  
31 open when fracturing fluid is withdrawn after a fracture treatment. ([U.S. EPA, 2013d](#))
- 32 **Protected ground water resource:** The deepest aquifer that the state or other regulatory agency  
33 requires to be protected from fluid migration through or along wellbores.

- 1 **Public water system source:** The source of the surface or ground water used by a public water  
2 system, including source wells, intakes, reservoirs, infiltration galleries, and springs.
- 3 **Public water systems:** Water systems that provide water for human consumption from surface or  
4 ground water through pipes or other infrastructure to at least 15 service connections or serve an  
5 average of at least 25 people for at least 60 days a year. ([Safe Drinking Water Act, 2002](#))
- 6 **Publicly owned treatment works (POTW):** Any device or system used in the treatment (including  
7 recycling and reclamation) of municipal sewage or industrial wastes of a liquid nature that is  
8 owned by a state or municipality. This definition includes sewers, pipes, or other conveyances only  
9 if they convey wastewater to a POTW providing treatment. ([U.S. EPA, 2013d](#))
- 10 **Quality assurance (QA):** An integrated system of management activities involving planning,  
11 implementation, documentation, assessment, reporting, and quality improvement to ensure that a  
12 process, item, or service is of the type and quality needed and expected by the customer. ([U.S. EPA,](#)  
13 [2013d](#))
- 14 **Quality assurance project plan (QAPP):** A formal document describing in comprehensive detail  
15 the necessary quality assurance procedures, quality control activities, and other technical activities  
16 that need to be implemented to ensure that the results of the work performed will satisfy the stated  
17 performance or acceptance criteria. ([U.S. EPA, 2013d](#))
- 18 **Quality management plan:** A document that describes a quality system in terms of the  
19 organizational structure, policy and procedures, functional responsibilities of management and  
20 staff, lines of authority, and required interfaces for those planning, implementing, documenting, and  
21 assessing all activities conducted. ([U.S. EPA, 2013d](#))
- 22 **Radioactive tracer log:** A record of the presence of tracer material placed in or around the  
23 borehole to measure fluid movement in injection wells. ([Schlumberger, 2014](#))
- 24 **Radionuclide:** Radioactive particle, man-made or natural, with a distinct atomic weight number.  
25 Emits radiation in the form of alpha or beta particles, or as gamma rays. Can have a long life as soil  
26 or water pollutant. Prolonged exposure to radionuclides increases the risk of cancer. ([U.S. EPA,](#)  
27 [2013d](#))
- 28 **Reference dose (RfD):** An estimate (with uncertainty spanning perhaps an order of magnitude) of  
29 a daily oral exposure to the human population (including sensitive subgroups) that is likely to be  
30 without an appreciable risk of deleterious effects during a lifetime.
- 31 **Reference value (RfV):** An estimate of an exposure for a given duration to the human population  
32 (including susceptible subgroups) that is likely to be without an appreciable risk of adverse health  
33 effects over a lifetime. Reference value is a generic term not specific to a given route of exposure.
- 34 **Relative permeability:** A dimensionless property allowing for comparison of the different abilities  
35 of fluids to flow in multiphase settings. If a single fluid is present, its relative permeability is equal

- 1 to 1, but the presence of multiple fluids generally inhibits flow and decreases the relative  
2 permeability.
- 3 **Reservoir:** A porous and permeable geologic formation where hydrocarbons collect under  
4 pressure over geological time.
- 5 **Residuals:** The solids generated or retained during the treatment of wastewater. ([U.S. EPA, 2013d](#))
- 6 **Safe Drinking Water Act (SDWA):** The act designed to protect the nation’s drinking water supply  
7 by establishing national drinking water standards (maximum contaminant levels or specific  
8 treatment techniques) and by regulating underground injection control wells. ([U.S. EPA, 2013d](#))
- 9 **Sandstone:** A clastic sedimentary rock whose grains are predominantly sand sized. The term is  
10 commonly used to imply consolidated sand or a rock made of predominantly quartz sand, although  
11 sandstones often contain feldspar, rock fragments, mica, and numerous additional mineral grains  
12 held together with silica or another type of cement. The relatively high porosity and permeability of  
13 sandstones make them good reservoir rocks. ([Schlumberger, 2014](#))
- 14 **Science Advisory Board (SAB):** A federal advisory committee that provides a balanced, expert  
15 assessment of scientific matters relevant to the EPA. An important function of the Science Advisory  
16 Board is to review EPA’s technical programs and research plans. ([U.S. EPA, 2013d](#))
- 17 **Service company:** A company that assists well operators by providing specialty services, including  
18 hydraulic fracturing. ([U.S. EPA, 2013d](#))
- 19 **Shale:** A fine-grained, fissile, detrital sedimentary rock formed by consolidation of clay- and silt-  
20 sized particles into thin, relatively impermeable layers. ([Schlumberger, 2014](#))
- 21 **Shale gas:** Natural gas generated and stored in shale.
- 22 **Shale oil:** Oil present in unconventional oil reservoirs that are made up of shale.
- 23 **Shut-in:** The process of sealing off a well by either closing the valves at the wellhead, a downhole  
24 safety valve, or a blowout preventer.
- 25 **Slickwater:** A type of fracturing fluid that consists mainly of water with a very low portion of  
26 additives like polymers that serve as friction reducers to reduce friction loss when pumping the  
27 fracturing fluid downhole. ([Barati and Liang, 2014](#))
- 28 **Solubility:** The amount of mass of a compound that will dissolve in a unit volume of solution. ([U.S.](#)  
29 [EPA, 2013d](#))
- 30 **Sorption:** The general term used to describe the partitioning of a chemical between soil and water  
31 and depends on the nature of the solids and the properties of the chemical.
- 32 **Source water:** Surface or ground water, or reused wastewater, acquired for use in hydraulic  
33 fracturing. ([U.S. EPA, 2013d](#))

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- 1 **Spacer fluid:** A fluid pumped before the cement to clean drilling mud out of the wellbore.
- 2 **Spud (spud a well):** To start the well drilling process by removing rock, dirt, and other  
3 sedimentary material with the drill bit. ([U.S. EPA, 2013d](#))
- 4 **Stages (frac stages):** A single reservoir interval that is hydraulically stimulated in succession with  
5 other intervals.
- 6 **Stimulation:** Refers to (1) injecting fluids to clear the well or pore spaces near the well of drilling  
7 mud or other materials that create blockage and inhibit optimal production (i.e., matrix treatment)  
8 and (2) injecting fluid to fracture the rock to optimize the production of oil or gas.
- 9 **Stray gas:** Refers to the phenomenon of natural gas (primarily methane) migrating into shallow  
10 drinking water resources or to the surface.
- 11 **Strings:** An assembled length of steel pipe configured to suit a specific wellbore.
- 12 **Subsurface formation:** A mappable body of rock of distinctive rock type(s), including the rock's  
13 pore volume (i.e., the void space within a formation that fluid flow can occur, as opposed to the bulk  
14 volume which includes both pore and solid phase volume), with a unique stratigraphic position.
- 15 **Surface casing:** The shallowest cemented casing, with the widest diameter. Cemented surface  
16 casing generally serves as an anchor for blowout protection equipment and to seal off drinking  
17 water resources. ([Baker, 1979](#))
- 18 **Surface water:** All water naturally open to the atmosphere (rivers, lakes, reservoirs, ponds,  
19 streams, impoundments, seas, estuaries, etc.). ([U.S. EPA, 2013d](#))
- 20 **Surfactant:** Used during the hydraulic fracturing process to decrease liquid surface tension and  
21 improve fluid passage through the pipes. ([U.S. EPA, 2013d](#))
- 22 **Sustained casing pressure:** Refers to cases when the pressure in any well annulus that is  
23 measurable at the wellhead rebuilds after it is bled down, not caused solely by temperature  
24 fluctuations or imposed by the operator. If the pressure is relieved by venting natural gas from the  
25 annulus to the atmosphere, it will build up again once the annulus is closed (i.e., the pressure is  
26 sustained). ([Skjerven et al., 2011](#))
- 27 **Technically recoverable resources:** The volumes of oil and natural gas that could be produced  
28 with current technology, regardless of oil and natural gas prices and production costs. ([EIA, 2013](#))
- 29 **Temperature log:** A log of the temperature of the fluids in the borehole; a differential temperature  
30 log records the rate of change in temperature with depth and is sensitive to very small changes.  
31 ([U.S. EPA, 2013d](#))
- 32 **Tensile strength:** The force per unit cross-sectional area required to pull a substance apart.  
33 ([Schlumberger, 2014](#))
-

- 1 **Thermogenic:** Methane that is produced by high temperatures and pressures in deep formations  
2 over geologic timescales. Thermogenic methane is formed by the thermal breakdown, or cracking,  
3 of organic material that occurs during deep burial of sediment.
- 4 **Tight oil:** Oil found in relatively impermeable reservoir rock. ([Schlumberger, 2014](#))
- 5 **Total dissolved solids (TDS):** The quantity of dissolved material in a given volume of water. Total  
6 dissolved solids can include salts (e.g., sodium chloride), dissolved metals, radionuclides, and  
7 dissolved organics. ([U.S. EPA, 2013d](#))
- 8 **Toxicity:** The degree to which a substance or mixture of substances can harm humans or animals.  
9 Acute toxicity involves harmful effects in an organism through a single or short-term exposure.  
10 Chronic toxicity is the ability of a substance or mixture of substances to cause harmful effects over  
11 an extended period, usually upon repeated or continuous exposure, sometimes lasting for the entire  
12 life of the exposed organism. Subchronic toxicity is the ability of the substance to cause effects for  
13 more than 1 year but less than the lifetime of the exposed organism. ([U.S. EPA, 2013d](#))
- 14 **Tubing:** The narrowest casing set within a completed well, either hung directly from the wellhead  
15 or secured at its bottom using a packer. Tubing is not typically cemented in the well.
- 16 **Unconventional reservoir:** A reservoir characterized by lower permeability than conventional  
17 reservoirs. It can be the same formation where hydrocarbons are formed and also serve as the  
18 source for hydrocarbons that migrate and accumulate in conventional reservoirs. Unconventional  
19 reservoirs can include methane-rich coalbeds and oil- and/or gas-bearing shales and tight sands.
- 20 **Unconventional resource:** An umbrella term for oil and natural gas that is produced by means  
21 that do not meet the criteria for conventional production. What has qualified as unconventional at  
22 any particular time is a complex function of resource characteristics, the available exploration and  
23 production technologies, the economic environment, and the scale, frequency, and duration of  
24 production from the resource. Perceptions of these factors inevitably change over time and often  
25 differ among users of the term. At present, the term is used in reference to oil and gas resources  
26 whose porosity, permeability, fluid trapping mechanism, or other characteristics differ from  
27 conventional sandstone and carbonate reservoirs. Coalbed methane, gas hydrates, shale gas,  
28 fractured reservoirs, and tight gas sands are considered unconventional resources. ([Schlumberger,  
29 2014](#))
- 30 **Underground Injection Control (UIC):** The program under the Safe Drinking Water Act that  
31 regulates the use of wells to pump fluids into the ground. ([U.S. EPA, 2013d](#))
- 32 **Unsaturated zone:** The soil zone above the water table that is only partially filled by water; also  
33 referred to as the “vadose zone.”
- 34 **Vapor pressure:** The force per unit area exerted by a vapor in an equilibrium state with its pure  
35 solid, liquid, or solution at a given temperature. Vapor pressure is a measure of a substance's

- 1 propensity to evaporate. Vapor pressure increases exponentially with an increase in temperature.  
2 ([U.S. EPA, 2013d](#))
- 3 **Vertical well:** A well in which the wellbore is vertical throughout its entire length, from the  
4 wellhead at the surface to the production zone.
- 5 **Viscosity:** A measure of the internal friction of a fluid that provides resistance to shear within the  
6 fluid, informally referred to as how "thick" a fluid is.
- 7 **Volatile:** Readily vaporizable at a relatively low temperature. ([U.S. EPA, 2013d](#))
- 8 **Volatilization:** The process in which a chemical leaves the liquid phase and enters the gas phase.
- 9 **Wastewater treatment:** Chemical, biological, and mechanical procedures applied to an industrial  
10 or municipal discharge or to any other sources of contaminated water in order to remove, reduce,  
11 or neutralize contaminants. ([U.S. EPA, 2013d](#))
- 12 **Water availability:** There is no standard definition for water availability, and it has not been  
13 assessed recently at the national scale ([U.S. GAO, 2014](#)). Instead, a number of water availability  
14 indicators have been suggested (e.g., [Roy et al., 2005](#)). Here, availability is most often used to  
15 qualitatively refer to the amount of a location's water that could, currently or in the future, serve as  
16 a source of drinking water ([U.S. GAO, 2014](#)), which is a function of water inputs to a hydrologic  
17 system (e.g., rain, snowmelt, groundwater recharge) and water outputs from that system occurring  
18 either naturally or through competing demands of users.
- 19 **Water consumption:** Water that is removed from the local hydrologic cycle following its use (e.g.,  
20 via evaporation, transpiration, incorporation into products or crops, consumption by humans or  
21 livestock), and is therefore unavailable to other water users ([Maupin et al., 2014](#)).
- 22 **Water intensity:** The amount of water used per unit of energy obtained. ([Nicot et al., 2014](#);  
23 [Laurenzi and Jersey, 2013](#))
- 24 **Water reuse:** Any hydraulic fracturing wastewater that is used to offset total fresh water  
25 withdrawals for hydraulic fracturing, regardless of the level of treatment required.
- 26 **Water use:** Water withdrawn for a specific purpose, part or all of which may be returned to the  
27 local hydrologic cycle.
- 28 **Water withdrawal:** Water removed from the ground or diverted from a surface-water source for  
29 use. ([Nicot et al., 2014](#); [Laurenzi and Jersey, 2013](#))
- 30 **Well blowout:** The uncontrolled flow of fluids out of a well.
- 31 **Well communication:** Refers to fractures intersecting abandoned or active (producing) offset  
32 wells near the well that is being stimulated.

- 1 **Well logging:** A continuous measurement of physical properties in or around the well with  
2 electrically powered instruments to infer formation properties. Measurements may include  
3 electrical properties (resistivity and conductivity), sonic properties, active and passive nuclear  
4 measurements, measurements of the wellbore, pressure measurement, formation fluid sampling,  
5 sidewall coring tools, and others. Measurements may be taken via a wireline, which is a wire or  
6 cable that is used to deploy tools and instruments downhole and that transmits data to the surface.  
7 ([Adapted from Schlumberger, 2014](#))
- 8 **Well operator:** A company that controls and operates oil and gas wells. ([U.S. EPA, 2013d](#))
- 9 **Well pad:** A temporary drilling site, usually constructed of local materials such as sand and gravel.  
10 After the drilling operation is over, most of the pad is usually removed or plowed back into the  
11 ground. ([NYSDEC, 2011](#))
- 12 **Wellbore:** The drilled hole or borehole, including the open hole or uncased portion of the well.
- 13 **Wet gas:** Refers to natural gas that typically contains less than 85% methane along with ethane and  
14 more complex hydrocarbons.
- 15 **Wetting/nonwetting:** The preferential attraction of a fluid to the surface. In typical reservoirs,  
16 water preferentially wets the surface, and gas is nonwetting. ([Adapted from Dake, 1978](#))
- 17 **Workover:** Refers to any maintenance activity performed on a well that involves ceasing  
18 operations and removing the wellhead.
- 19 **Young's modulus:** A ratio of stress to strain that is a measure of the rigidity of a material.

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