A 01

CODING FORMS FOR SRC INDEXING

Microfiche No.		
OTS0559902		
New Doc ID	Old Doc ID	
88000000141	8EHQ-0400-14702	
Date Produced	Date Received	TSCA Section
07/01/91	04/18/00	8E
Submitting Organization		
TCC CONSORTIUM		
Contractor		
BAYER AG		
Document Title		
INITIAL SUBMISSION: PREVENTOL SB (TRICLOCARBAN) - DETERMINATION OF KOW, AND QSAR ANALYSIS/EPIWIN MODELING DETERMINATION OF BCF, WITH TSCA HLTH & SFTY STUDY CVR SHT DATED 4/12/00		
Chemical Category		
UREA, N-(4-CHLOROPHENYL)-N'-(3,4-DICHLOROPHENYL)-		

A 03

8EHQ-0400-14702

T SCA HEALTH & SAFETY STUDY COVER SHEET

TSCA CBI STATUS:

☐ CHECK IF THIS PAGE CONTAINS CONFIDENTIAL BUSINESS INFORMATION (CBI)

Clearly mark the confidential information with bracketing and check the box in the appropriate section (☐ *Contains CBI*). Submit a sanitized cover sheet with CBI deleted. Mark the sanitized copy, "Public Display Copy" in the heading.

1.0 SUBMISSION TYPE ☐ *Contains CBI*

☐ 8(d) ☐ 8(c) ☐ FYI ☐ 4 ☒ OTHER: Specify ITC

☒ Intial Submission ☐ Follow-up Submission ☐ Final Report Submission

Previous EPA Submission Number or Title if update or follow-up: Docket Number, if any: #

☒ continuation sheet attached

2.1 SUMMARY/ABSTRACT ATTACHED (may be required for 8(e): optional for §4, 8(d) & FYI)	2.2 SUBMITTER TRACKING NUMBER OR INTERNAL ID	2.3 FOR EPA USE ONLY
☒ YES ☐ NO	P 917 006 961 A90/00665/01	

3.0 CHEMICAL/TEST SUBSTANCE IDENTITY ☐ *Contains CBI*

Reported Chemical Name (specify nomenclature if other than CAS name):

CAS# 101-20-2 Urea, N-(4-Chlorophenyl)-N'-(3,4-dichlorophenyl)-

Purity ____ %

☐ Single Ingredient

☒ Commerical/Tech Grade

☐ Mixture *Trade Name:* Preventol SB *Common Name:* triclocarban

CAS Number	*NAME*	*% WEIGHT*

Other chemical(s) present in tested mixture

☐ continuation sheet attached

4.0 REPORT/STUDY TITLE ☐ *Contains CBI*

Partition Coefficient

8EHQ-00-14702

☐ continuation sheet attached

5.1 STUDY/TSCATS INDEXING TERMS

[CHECK ONE]

HEALTH EFFECTS (HE): ____ ENVIRONMENTAL EFFECTS (EE): ____ ENVIRONMENTAL FATE (EF): X

5.2 STUDY/TSCATS INDEXING TERMS (see instructions for 4 digit codes)

STUDY TYPE: LogP SUBJECT ORGANISM (HE, EE only): ____ ROUTE OF EXPOSURE (HE only): ____ VEHICLE OF EXPOSURE (HE only) ____

Other: ____ *Other:* ____ *Other:* ____ *Other:* ____

6.0 REPORT/STUDY INFORMATION ☐ *Contains CBI* ☒ Study is GLP

Laboratory Bayer AG Report/Study Date 7/1/91

Source of Data/Study Sponsor (if different than submitter) Bayer AG Number of pages 4

☐ continuation sheet attached

7.0 SUBMITTER INFORMATION ☐ *Contains CBI*

Submitter: TCC Consortium Title: Alvaro J. DeCarvalho, Consortium Manager Phone: (212) 725-1262

Company Name: Soap and Detergent Association Company Address: 475 Park Avenue South

New York, NY 10016 Submitter Address (if different): ____

Technical Contact: Cynthia Graham, Ph.D. Phone: (412) 777-3933

☐ continuation sheet attached

8.0 ADDITIONAL/OPTIONAL STUDY COMMENTS ☐ *Contains CBI*

The EPIWIN modeling summary for TCC is attached. The BCF was calculated, using the experimental logP = 4.2.

☐ continuation sheet attached

CONTAINS NO CBI

Submitter Signature: Alvaro J. DeCarvalho / cg **Date:** 4/12/00

MR 34852

RECEIVED OPPT NCIC 2000 APR 18 AM 11:42

CONTAINS NO CBI

RECEIVED OPPT NCIC 2000 MAY -5 PM 4:56

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A 04

TSCA HEALTH & SAFETY STUDY COVER SHEET - revised 6/25/96

9.0 CONTINUATION SHEET

TSCA CBI STATUS:

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Submitter Tracking Number/Internal ID

P 917 006 961
A90/00665/01

CONTINUED FROM COVER SHEET SECTION # 2.1

☐ *Contains CBI*

The determination of the Partition coefficient was done in a Bayer AG lab in 1991, using HPLC and in accordance with GLP procedures. The log P (octanol/ water) = 4.2

QSAR analysis (using the EPIWIN modeling program) has shown that TCC has a BCF < 500 which would classify it as non-bioaccumulative by the draft OECD Guideline ENV/MC/CHEM/HCL(98)15/REV2: A Harmonized Integrated Hazard Classification System for Human Health and Environmental Effects of Chemicals; Chapter: Harmonized system for classification of chemicals which are hazardous for the aquatic environment.

Final Report

DISTRIBUTION COEFFICIENT

BAYER AG
ZF-D/Central Analysis
Bldg. O 13
5090 Leverkusen

Date : July 1, 1991
Study Number : A 90/0065/01 LEV
Study Director : Dr. Klein
Assistant : Dr. Kassühlke

Test substance: Preventol SB powder

Customer: Dr. A. Paetz, BALK, Lev., D 8 Order Number: 90/060

Chemical name : 3,4,4'-trichlorocarbanilide
Empirical formula : $C_{13}H_9Cl_3N_2O$ Molar mass : 315.6 g/mole
CAS name : Urea, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-
CAS No. : 101-20-2
Product No. : 066 111 00 Batch No. : 19
Sample No. : 81733/1990 Sampling date : 08.05.90
Production plant : PHN plant Production date : 09.11.89
Expires : 08.05.92
Start of study : 16.05.91
End of study : 21.06.91

1. Description of the methods and individual results

1.1 Test : Distribution coefficient P (in n-octanol/water)
SOP : AXX 0002202
SOP : A 0002102 (additional information)
SOP : FXX 0002901 (pH value)

Method : K2011-0209601-91D (HPLC assay)
Lab. Manager : Dr. Reusche
Dr. Klein

Result : See table

Final Report

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Test substance: Preventol SB powder

Customer: Dr. A. Paetz, BALK, Lev., D 8 Order Number: 90/060

Result

Test No.	pH value of water phase	Volume Octanol Phase (ml)	Volume Water phase (ml)	Concentration Octanol phase (mg/ml)	Concentration Water phase (mg/ml)	Dist. coeff. Indiv.	Dist. coeff. Mean
1a	5.6	5.0	245.0	2.0	$125*10^{-6}$	16000	
1b	5.6	5.0	245.0	2.0	$104*10^{-6}$	19231	17616
2a	5.6	10.0	240.0	1.0	$59*10^{-6}$	16949	
2b	5.6	10.0	240.0	1.0	$61*10^{-6}$	16393	16671
3a	5.6	20.0	230.0	0.5	$38*10^{-6}$	13158	
3b	5.6	20.0	230.0	0.5	$29*10^{-6}$	17241	15200

Quantity of test substance used : 10.00 mg/batch

Test temperature : 22.6 °C ± 1 °C

pH of water : 6.1

Distribution coefficient P : $1.6*10^4$

log P : 4.2

Sp (abs. standard deviation) : $2*10^3$

Final Report

DISTRIBUTION COEFFICIENT

BAYER AG
ZF-D/Central Analysis
Bldg. O 13
5090 Leverkusen

Date : July 1, 1991
Study Number : A 90/0065/01 LEV
Study Director : Dr. Klein
Assistant : Dr. Kassühlke

Test substance: Preventol SB powder

Customer: Dr. A. Paetz, BALK. Lev., D 8 Order Number: 90/060

2. **Assessment and comments**

- The raw data have been examined and archived.

3. **Declaration**

The study was conducted according to the OECD principles of Good Laboratory Practice (GLP).

4. **Archiving**

The study protocol and the other test documentation are filed in the archive of ZF-DZA/OAL, BAYER AG Leverkusen, Bldg. O 13.

Leverkusen, July 1, 1991

Study director : (signed)

Laboratory director : (signed), 01.10.91
(Dr. Reusche)

Enclosures: Declaration of the Quality Assurance Unit (QAU)

Copies to: Dr. A. Paetz, Bayer Altstoffkommission LEV, Bldg. D 8
Archive
Head of Test Centre
QAU
ZF-DZA Koordination Alt- und Neustoffanalytik
Dr. Winkler, OC-P/PHN LEV, Bldg. O 18
Dr. Neuhahn, OC-P/Oek LEV, Bldg. G 19
Dr. Klein

BAYER AG
ZF-D/Central Analysis Leverkusen/OAL
Bldg. O 13
5090 Leverkusen 1

Quality assurance declaration for Final Report

Study No. or Order No.: A90/0065/01 LEV
Title of GLP study: Distribution coefficient of Preventol SB powder

This GLP study was continuously monitored by Quality Assurance. The dates of inspection and the dates of the reports to the Head of the Test Centre and to the Study Director are listed below.

Inspection (Date)	Report (Date)
14.05.91	14.05.91
17.06.91	17.06.91
07.10.91	07.10.91
14.10.91	14.10.91

The results presented in the Final Report of this study were checked according to current SOPs/Analysis Methods. To the best of our knowledge, they correspond to the available raw data.

Quality Assurance:

Oct. 14, 91
(Date)

(signed)
(WILLERS)

A 09


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SMILES : O=C(Nc(ccc(c1)CL)c1)Nc(ccc(c2CL)CL)c2
CHEM   : Urea, N-(4-chlorophenyl)-N'-(3,4-dichlorophenyl)-
CAS NUM: 000101-20-2
MOL FOR: C13 H9 CL3 N2 O1
MOL WT : 315.59
----------------------------EPI SUMMARY (v3.04)----------------
 Physical Property Inputs:
    Water Solubility (mg/L):    ------
    Vapor Pressure (mm Hg) :    ------
    Henry LC (atm-m3/mole) :    ------
    Log Kow (octanol-water):    4.20
    Boiling Point (deg C)  :    ------
    Melting Point (deg C)  :    ------

 Log Octanol-Water Partition Coef (SRC):
    Log Kow (KOWWIN v1.65 estimate) =  4.90

 Boiling Pt, Melting Pt, Vapor Pressure Estimations
(MPBPWIN v1.31):
    Boiling Pt (deg C):  434.57  (Adapted Stein & Brown method)
    Melting Pt (deg C):  182.04  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  2.73E-008  (Modified Grain method)

 Water Solubility Estimate from Log Kow (WSKOW v1.36):
    Water Solubility at 25 deg C (mg/L):  2.575
       log Kow used: 4.20 (user entered)
       no-melting pt equation used

 ECOSAR Class Program (ECOSAR v0.99e):
    Class(es) found:
       Neutral Organics
       Ureas(substituted)

 Henrys Law Constant (25 deg C) [HENRYWIN v3.04]:
   Bond Method :   4.52E-011  atm-m3/mole
   Group Method:   Incomplete
 Henrys LC [VP/WSol estimate using EPI values]:  4.402E-009 atm-
m3/mole

 Probability of Rapid Biodegradation (BIOWIN v3.67):
    Linear Model         :   0.0500
    Non-Linear Model     :   0.0005
 Expert Survey Biodegradation Results:
    Ultimate Survey Model:   1.8820  (months      )
    Primary Survey Model :   2.8964  (weeks       )
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Atmospheric Oxidation (25 deg C) [AopWin v1.89]:
   Hydroxyl Radicals Reaction:
      OVERALL OH Rate Constant =  21.2164 E-12 cm3/molecule-sec
      Half-Life =     0.504 Days (12-hr day; 1.5E6 OH/cm3)
      Half-Life =     6.050 Hrs
   Ozone Reaction:
      No Ozone Reaction Estimation

 Soil Adsorption Coefficient (PCKOCWIN v1.66):
      Koc    :  5394
      Log Koc:  3.732

 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C)
[HYDROWIN v1.67]:
    Rate constants can NOT be estimated for this structure!

 BCF Estimate from Log Kow (BCFWIN v2.13):
    Log BCF =  2.534   (BCF = 342)
       log Kow used: 4.20 (user entered)

 Volatilization from Water:
    Henry LC:  4.52E-011 atm-m3/mole  (estimated by Bond SAR
Method)
    Half-Life from Model River: 2.301E+007  hours   (9.588E+005
days)
    Half-Life from Model Lake :  2.51E+008  hours   (1.046E+007
days)

 Removal In Wastewater Treatment:
    Total removal:              39.94  percent
    Total biodegradation:        0.40  percent
    Total sludge adsorption:    39.54  percent
    Total to Air:                0.00  percent

 Level III Fugacity Model:
          Concentration   Half-Life    Emissions
            (percent)        (hr)        (kg/hr)
   Air      0.000727        12.1         1000
   Water    14.9            1.44e+003    1000
   Soil     80.6            1.44e+003    1000
   Sediment 4.5             5.76e+003    0
     Persistence Time: 1.63e+003 hr
```