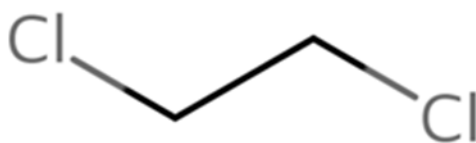


## Risk Evaluation for 1,2-Dichloroethane

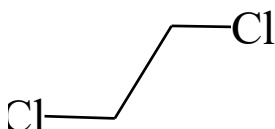
### Supplemental Information File:

### Supplemental Information on EPI Suite Modeling Results in the Fate Assessment

**CASRN 107-06-2**



EPI Suite Results For CAS 107-06-2



SMILES : CLCCCL  
 CHEM : Ethane, 1,2-dichloro-  
 MOL FOR: C2 H4 CL2  
 MOL WT : 98.96

----- EPI SUMMARY (v4.11) -----

Physical Property Inputs:  
 Log Kow (octanol-water): 1.48  
 Boiling Point (deg C) : 83.43  
 Melting Point (deg C) : -35.61  
 Vapor Pressure (mm Hg) : 78.9  
 Water Solubility (mg/L): 8600  
 Henry LC (atm-m3/mole) : 0.00154

KOWWIN Program (v1.68) Results:

=====

Log Kow(version 1.69 estimate): 1.83

Experimental Database Structure Match:

Name : 1,2-DICHLOROETHANE  
 CAS Num : 000107-06-2  
 Exp Log P: 1.48  
 Exp Ref : HANSCH,C ET AL. (1995)

SMILES : CLCCCL  
 CHEM : Ethane, 1,2-dichloro-  
 MOL FOR: C2 H4 CL2  
 MOL WT : 98.96

| TYPE | NUM | LOGKOW | FRAGMENT DESCRIPTION | COEFF | VALUE |
|------|-----|--------|----------------------|-------|-------|
|------|-----|--------|----------------------|-------|-------|



| TYPE   | NUM | MELT DESCRIPTION            | COEFF | VALUE   |
|--------|-----|-----------------------------|-------|---------|
| Group  | 2   | -CH2-                       | 11.27 | 22.54   |
| Group  | 2   | -Cl (primary)               | 13.55 | 27.10   |
| *      |     | Equation Constant           |       | 122.50  |
| =====  |     |                             |       |         |
| RESULT |     | MELTING POINT in deg Kelvin |       | 172.14  |
|        |     | MELTING POINT in deg C      |       | -101.02 |

Water Sol from Kow (WSKOW v1.42) Results:

Water Sol: 9056 mg/L

Experimental Water Solubility Database Match:

Name : 1,2-DICHLOROETHANE  
CAS Num : 000107-06-2  
Exp WSol : 8600 mg/L (25 deg C)  
Exp Ref : HORVATH,AL ET AL. (1999)

Experimental Water Solubility Database Match:

Name : DICHLOROETHANES  
CAS Num : 001300-21-6  
Exp WSol : 5100 mg/L ( deg C)  
Exp Ref : KUHN,W & SANDER,R (1981)

SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96

----- WSKOW v1.43 Results -----

Log Kow (estimated) : 1.83  
Log Kow (experimental): 1.48  
Cas No: 000107-06-2  
Name : 1,2-DICHLOROETHANE  
Refer : HANSCH,C ET AL. (1995)  
Log Kow used by Water solubility estimates: 1.48 (user entered)

Equation Used to Make Water Sol estimate:

$\text{Log S (mol/L)} = 0.693 - 0.96 \log \text{Kow} - 0.0092(\text{Tm} - 25) - 0.00314 \text{ MW} + \text{Correction}$

Melting Pt (Tm) = -35.61 deg C (Use Tm = 25 for all liquids)

Correction(s): Value

-----  
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -1.039  
Water Solubility at 25 deg C (mg/L): 9056

WATERNT Program (v1.01) Results:

=====

Water Sol (v1.01 est): 3946.8 mg/L

Experimental Water Solubility Database Match:

Name : 1,2-DICHLOROETHANE  
CAS Num : 000107-06-2  
Exp WSol : 8600 mg/L (25 deg C)  
Exp Ref : HORVATH,AL ET AL. (1999)

Experimental Water Solubility Database Match:

Name : DICHLOROETHANES  
CAS Num : 001300-21-6  
Exp WSol : 5100 mg/L ( deg C)  
Exp Ref : KUHN,W & SANDER,R (1981)

SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96

| TYPE  | NUM | WATER SOLUBILITY FRAGMENT DESCRIPTION | COEFF   | VALUE   |
|-------|-----|---------------------------------------|---------|---------|
| Frag  | 2   | -CH2- [aliphatic carbon]              | -0.5370 | -1.0740 |
| Frag  | 2   | -CL [chlorine, aliphatic attach]      | -0.2872 | -0.5744 |
| Const |     | Equation Constant                     |         | 0.2492  |

Log Water Sol (moles/L) at 25 dec C = -1.3992  
Water Solubility (mg/L) at 25 dec C = 3946.8

ECOSAR Program (v1.11) Results:

=====  
ECOSAR Version 1.11 Results Page

SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
CAS Num:  
ChemID1:  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96  
Log Kow: 1.832 (EPISuite Kowwin v1.68 Estimate)  
Log Kow: (User Entered)  
Log Kow: 1.48 (PhysProp DB exp value - for comparison only)  
Melt Pt: -35.61 (deg C, UserEntered for Wat Sol estimate)  
Melt Pt: -35.50 (deg C, PhysProp DB exp value for Wat Sol est)  
Wat Sol: 9056 (mg/L, EPISuite WSKowwin v1.43 Estimate)  
Wat Sol: 8600 (mg/L, User Entered)  
Wat Sol: 5100 (mg/L, PhysProp DB exp value)

-----  
Values used to Generate ECOSAR Profile  
-----

Log Kow: 1.832 (EPISuite Kowwin v1.68 Estimate)  
Wat Sol: 8600 (mg/L, User Entered)

-----  
ECOSAR v1.11 Class-specific Estimations  
-----

Neutral Organics

Predicted

| ECOSAR Class     | Organism      | Duration | End Pt | mg/L (ppm) |
|------------------|---------------|----------|--------|------------|
| Neutral Organics | : Fish        | 96-hr    | LC50   | 115.160    |
| Neutral Organics | : Daphnid     | 48-hr    | LC50   | 64.380     |
| Neutral Organics | : Green Algae | 96-hr    | EC50   | 44.970     |
| Neutral Organics | : Fish        |          | ChV    | 11.052     |
| Neutral Organics | : Daphnid     |          | ChV    | 6.012      |
| Neutral Organics | : Green Algae |          | ChV    | 11.376     |
| Neutral Organics | : Fish (SW)   | 96-hr    | LC50   | 144.831    |
| Neutral Organics | : Mysid       | 96-hr    | LC50   | 120.644    |
| Neutral Organics | : Fish (SW)   |          | ChV    | 14.184     |
| Neutral Organics | : Mysid (SW)  |          | ChV    | 10.962     |
| Neutral Organics | : Earthworm   | 14-day   | LC50   | 179.112    |

Note: \* = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

-----  
 Class Specific LogKow Cut-Offs  
 -----

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Neutral Organics:  
 -----

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)  
 Maximum LogKow: 6.0 (Earthworm LC50)  
 Maximum LogKow: 6.4 (Green Algae EC50)  
 Maximum LogKow: 8.0 (ChV)

HENRYWIN (v3.20) Program Results:  
 =====

Bond Est : 1.21E-002 atm-m3/mole (1.23E+003 Pa-m3/mole)  
 Group Est: 1.94E-004 atm-m3/mole (1.97E+001 Pa-m3/mole)

SMILES : CLCCCL  
 CHEM : Ethane, 1,2-dichloro-  
 MOL FOR: C2 H4 CL2  
 MOL WT : 98.96

----- HENRYWIN v3.21 Results -----

Experimental Database Structure Match:

Name : 1,2-DICHLOROETHANE  
 CAS Num : 000107-06-2  
 Exp HLC : 1.18E-03 atm-m3/mole (120 Pa-m3/mole)  
 Temper : 25 deg C  
 Exp Ref : LEIGHTON,DTJR & CALO,JM (1981)

-----+-----+-----+-----  
 CLASS | BOND CONTRIBUTION DESCRIPTION | COMMENT | VALUE

|          |  |   |                                      |  |  |  |         |
|----------|--|---|--------------------------------------|--|--|--|---------|
| HYDROGEN |  | 4 | Hydrogen to Carbon (aliphatic) Bonds |  |  |  | -0.4787 |
| FRAGMENT |  | 1 | C-C                                  |  |  |  | 0.1163  |
| FRAGMENT |  | 2 | C-CL                                 |  |  |  | 0.6669  |

|        |  |  |  |  |  |  |       |  |       |
|--------|--|--|--|--|--|--|-------|--|-------|
| RESULT |  | BOND ESTIMATION METHOD for LWAPC VALUE |  |  |  |  | TOTAL |  | 0.305 |
|--------|--|--|--|--|--|--|-------|--|-------|

HENRYs LAW CONSTANT at 25 deg C = 1.21E-002 atm-m3/mole  
= 4.96E-001 unitless  
= 1.23E+003 Pa-m3/mole

| GROUP CONTRIBUTION DESCRIPTION | COMMENT | VALUE |
|--------------------------------|---------|-------|
| 2 CH2 (C) (CL)                 |         | 2.10  |

|        |  |   |  |  |       |  |      |
|--------|--|---|--|--|-------|--|------|
| RESULT |  | GROUP ESTIMATION METHOD for LOG GAMMA VALUE |  |  | TOTAL |  | 2.10 |
|--------|--|---|--|--|-------|--|------|

HENRYs LAW CONSTANT at 25 deg C = 1.94E-004 atm-m3/mole  
= 7.94E-003 unitless  
= 1.97E+001 Pa-m3/mole

For Henry LC Comparison Purposes:

Exper Database: 1.18E-03 atm-m3/mole (1.20E+002 Pa-m3/mole)  
User-Entered Henry LC: 1.540E-003 atm-m3/mole (1.560E+002 Pa-m3/mole)  
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:  
HLC: 1.195E-003 atm-m3/mole (1.210E+002 Pa-m3/mole)  
VP: 78.9 mm Hg (source: User-Entered)  
WS: 8.6E+003 mg/L (source: User-Entered)

Log Octanol-Air (KOAWIN v1.10) Results:

Log Koa: 2.681

SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96

----- KOAWIN v1.10 Results -----

Experimental Database Structure Match:

Name : 1,2-Dichloroethane  
CAS Num : 000107-06-2  
Exp LogKoa: 2.78  
Exp Ref : Abraham,MH et al. (2001)

Log Koa (octanol/air) estimate: 2.681

Koa (octanol/air) estimate: 479.7

Using:

Log Kow: 1.48 (user entered)  
HenryLC: 0.00154 atm-m3/mole (user entered)  
Log Kaw: -1.201 (air/water part.coef.)

LogKow : 1.48 (exp database)

LogKow : 1.83 (KowWin estimate)

Henry LC: 0.00118 atm-m3/mole (exp database)

Henry LC: 0.0121 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 2.136 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:

SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast  
Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast  
Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months  
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks  
Biowin5 (MITI Linear Model Prediction) : Does Not Biodegrade Fast  
Biowin6 (MITI Non-Linear Model Prediction): Does Not Biodegrade Fast  
Biowin7 (Anaerobic Model Prediction): Biodegrades Fast  
Ready Biodegradability Prediction: NO

| TYPE   | NUM | Biowin1 FRAGMENT DESCRIPTION        | COEFF   | VALUE   |
|--------|-----|-------------------------------------|---------|---------|
| Frag   | 2   | Aliphatic chloride [-CL]            | -0.1114 | -0.2228 |
| MolWt  | *   | Molecular Weight Parameter          |         | -0.0471 |
| Const  | *   | Equation Constant                   |         | 0.7475  |
| RESULT |     | Biowin1 (Linear Biodeg Probability) |         | 0.4777  |

| TYPE   | NUM | Biowin2 FRAGMENT DESCRIPTION            | COEFF   | VALUE   |
|--------|-----|---|---------|---------|
| Frag   | 2   | Aliphatic chloride [-CL]                | -1.8528 | -3.7056 |
| MolWt  | *   | Molecular Weight Parameter              |         | -1.4052 |
| RESULT |     | Biowin2 (Non-Linear Biodeg Probability) |         | 0.1089  |

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

| TYPE   | NUM | Biowin3 FRAGMENT DESCRIPTION             | COEFF   | VALUE   |
|--------|-----|--|---------|---------|
| Frag   | 2   | Aliphatic chloride [-CL]                 | -0.1732 | -0.3464 |
| MolWt  | *   | Molecular Weight Parameter               |         | -0.2187 |
| Const  | *   | Equation Constant                        |         | 3.1992  |
| RESULT |     | Biowin3 (Survey Model - Ultimate Biodeg) |         | 2.6341  |

| TYPE  | NUM | Biowin4 FRAGMENT DESCRIPTION | COEFF   | VALUE   |
|-------|-----|------------------------------|---------|---------|
| Frag  | 2   | Aliphatic chloride [-CL]     | -0.1006 | -0.2012 |
| MolWt | *   | Molecular Weight Parameter   |         | -0.1428 |

|        |   |   |  |        |
|--------|---|---|--|--------|
| Const  | * | Equation Constant                       |  | 3.8477 |
| =====  |   |   |  |        |
| RESULT |   | Biowin4 (Survey Model - Primary Biodeg) |  | 3.5037 |
| =====  |   |   |  |        |

Result Classification: 5.00 -> hours      4.00 -> days      3.00 -> weeks  
 (Primary & Ultimate)      2.00 -> months      1.00 -> longer

| TYPE   | NUM | Biowin5 FRAGMENT DESCRIPTION             | COEFF  | VALUE   |
|--------|-----|--|--------|---------|
| Frag   | 2   | Aliphatic chloride [-CL]                 | 0.0174 | 0.0349  |
| Frag   | 2   | -CH2- [linear]                           | 0.0255 | 0.0511  |
| MolWt  | *   | Molecular Weight Parameter               |        | -0.1561 |
| Const  | *   | Equation Constant                        |        | 0.5544  |
| =====  |     |  |        |         |
| RESULT |     | Biowin5 (MITI Linear Biodeg Probability) |        | 0.4842  |
| =====  |     |  |        |         |

| TYPE   | NUM | Biowin6 FRAGMENT DESCRIPTION                 | COEFF   | VALUE   |
|--------|-----|--|---------|---------|
| Frag   | 2   | Aliphatic chloride [-CL]                     | -0.6392 | -1.2784 |
| Frag   | 2   | -CH2- [linear]                               | 0.2345  | 0.4690  |
| MolWt  | *   | Molecular Weight Parameter                   |         | -1.7120 |
| =====  |     |  |         |         |
| RESULT |     | Biowin6 (MITI Non-Linear Biodeg Probability) |         | 0.2975  |
| =====  |     |  |         |         |

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

| TYPE   | NUM | Biowin7 FRAGMENT DESCRIPTION           | COEFF   | VALUE   |
|--------|-----|--|---------|---------|
| Frag   | 2   | Aliphatic chloride [-CL]               | -0.0147 | -0.0293 |
| Frag   | 2   | -CH2- [linear]                         | 0.0260  | 0.0520  |
| Const  | *   | Equation Constant                      |         | 0.8361  |
| =====  |     |  |         |         |
| RESULT |     | Biowin7 (Anaerobic Linear Biodeg Prob) |         | 0.8587  |
| =====  |     |  |         |         |

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is  $\geq 0.5$ , then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERI/J) database.

BioHCwin (v1.01) Program Results:

=====  
SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96

----- BioHCwin v1.01 Results -----

NO Estimate Possible ... Structure NOT a Hydrocarbon  
(Contains atoms other than C, H or S (-S-))

AEROWIN Program (v1.00) Results:

=====  
Sorption to aerosols (25 Dec C) [AEROWIN v1.00]:  
Vapor pressure (liquid/subcooled): 1.05E+004 Pa (78.9 mm Hg)  
Log Koa (Exp database): 2.780  
Kp (particle/gas partition coef. (m3/ug)):  
Mackay model : 2.85E-010  
Octanol/air (Koa) model: 1.48E-010  
Fraction sorbed to airborne particulates (phi):  
Junge-Pankow model : 1.03E-008  
Mackay model : 2.28E-008  
Octanol/air (Koa) model: 1.18E-008

AOP Program (v1.92) Results:

=====  
SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96

----- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) -----

Hydrogen Abstraction = 0.2555 E-12 cm3/molecule-sec  
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec  
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec  
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec  
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec  
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 0.2555 E-12 cm3/molecule-sec  
HALF-LIFE = 41.856 Days (12-hr day; 1.5E6 OH/cm3)

----- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----

\*\*\*\*\* NO OZONE REACTION ESTIMATION \*\*\*\*\*  
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database Structure Match:

Chem Name : 1,2-DICHLOROETHANE  
CAS Number: 000107-06-2  
Exper OH rate constant : 0.248 E-12 cm3/molecule-sec  
Exper OH Reference: KWOK,ESC & ATKINSON,R (1994)  
Exper Ozone rate constant: --- cm3/molecule-sec  
Exper NO3 rate constant : --- cm3/molecule-sec  
Fraction sorbed to airborne particulates (phi):  
1.66E-008 (Junge-Pankow, Mackay avg)  
1.18E-008 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

KOCWIN Program (v2.00) Results:

SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96

Experimental Database Structure Match:

Name : 1,2-Dichloroethane  
CAS Num : 000107-06-2  
Exp LogKoc: 1.52  
Exp Ref : SRC (1991); Meylan et al (1992)

KOCWIN v2.01 Results

Koc Estimate from MCI:

First Order Molecular Connectivity Index : 1.914  
Non-Corrected Log Koc (0.5213 MCI + 0.60) : 1.5977  
Fragment Correction(s) --> NONE : ---  
Corrected Log Koc : 1.5977

Estimated Koc: 39.6 L/kg <=====

Koc Estimate from Log Kow:

Log Kow (User entered ) : 1.48  
Non-Corrected Log Koc (0.8679 logKow - 0.0004) : 1.2841  
Fragment Correction(s) --> NONE : ---  
Corrected Log Koc : 1.2841

Estimated Koc: 19.23 L/kg <=====

HYDROWIN Program (v2.00) Results:

SMILES : CLCCCL  
CHEM : Ethane, 1,2-dichloro-  
MOL FOR: C2 H4 CL2  
MOL WT : 98.96

HYDROWIN v2.00 Results

R2

| X: -CL (Leaving halogen in R1)  
ALKYL HALIDE: R1-C-H R1: -CH2-CL

| R2: -CL

R3 R3: -H

Kb hydrolysis at atom # 3: 4.686E-007 L/mol-sec

Total Kb for pH > 8 at 25 deg C : 4.686E-007 L/mol-sec

Kb Half-Life at pH 8: 4.687E+004 years

Kb Half-Life at pH 7: 4.687E+005 years

The rate constant estimated for the ALKYL HALIDE DOES NOT include the neutral hydrolysis rate constant!!  
 For some alkyl halides, the neutral rate constant is the dominant hydrolysis rate at environmental pHs!  
 If the neutral rate constant is important, the HYDRO estimated rate will under-estimate the actual rate!

BCFBFAF Program (v3.01) Results:

=====

SMILES : CLCCCL  
 CHEM : Ethane, 1,2-dichloro-  
 MOL FOR: C2 H4 CL2  
 MOL WT : 98.96

----- BCFBAF v3.01 -----

Summary Results:

Log BCF (regression-based estimate): 0.64 (BCF = 4.4 L/kg wet-wt)  
 Biotransformation Half-Life (days) : 0.272 (normalized to 10 g fish)  
 Log BAF (Arnot-Gobas upper trophic): 0.58 (BAF = 3.78 L/kg wet-wt)

Log Kow (experimental): 1.48  
 Log Kow used by BCF estimates: 1.48 (user entered)

Equation Used to Make BCF estimate:  
 Log BCF = 0.6598 log Kow - 0.333 + Correction

Correction(s): Value  
 No Applicable Correction Factors

Estimated Log BCF = 0.644 (BCF = 4.401 L/kg wet-wt)

=====

Whole Body Primary Biotransformation Rate Estimate for Fish:

| TYPE   | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION        | COEFF  | VALUE   |
|--------|-----|---|--------|---------|
| Frag   | 2   | Aliphatic chloride [-CL]                          | 0.3608 | 0.7215  |
| Frag   | 2   | -CH2- [linear]                                    | 0.0242 | 0.0484  |
| L Kow  | *   | Log Kow = 1.48 (user-entered )                    | 0.3073 | 0.4549  |
| MolWt  | *   | Molecular Weight Parameter                        |        | -0.2538 |
| Const  | *   | Equation Constant                                 |        | -1.5371 |
| RESULT |     | LOG Bio Half-Life (days)                          |        | -0.5661 |
| RESULT |     | Bio Half-Life (days)                              |        | 0.2716  |
| NOTE   |     | Bio Half-Life Normalized to 10 g fish at 15 deg C |        |         |

Biotransformation Rate Constant:  
 kM (Rate Constant): 2.552 /day (10 gram fish)  
 kM (Rate Constant): 1.435 /day (100 gram fish)  
 kM (Rate Constant): 0.807 /day (1 kg fish)  
 kM (Rate Constant): 0.4538 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):  
 Estimated Log BCF (upper trophic) = 0.577 (BCF = 3.777 L/kg wet-wt)  
 Estimated Log BAF (upper trophic) = 0.577 (BAF = 3.777 L/kg wet-wt)  
 Estimated Log BCF (mid trophic) = 0.461 (BCF = 2.89 L/kg wet-wt)

Estimated Log BAF (mid trophic) = 0.461 (BAF = 2.89 L/kg wet-wt)  
 Estimated Log BCF (lower trophic) = 0.426 (BCF = 2.669 L/kg wet-wt)  
 Estimated Log BAF (lower trophic) = 0.426 (BAF = 2.67 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):  
 Estimated Log BCF (upper trophic) = 0.615 (BCF = 4.123 L/kg wet-wt)  
 Estimated Log BAF (upper trophic) = 0.621 (BAF = 4.176 L/kg wet-wt)

Volatilization From Water  
 =====

Chemical Name: Ethane, 1,2-dichloro-

Molecular Weight : 98.96 g/mole  
 Water Solubility : 8600 ppm  
 Vapor Pressure : 78.9 mm Hg  
 Henry's Law Constant: 0.00154 atm-m<sup>3</sup>/mole (entered by user)

| RIVER                     | LAKE          |
|---------------------------|---------------|
| -----                     | -----         |
| Water Depth (meters):     | 1             |
| Wind Velocity (m/sec):    | 0.5           |
| Current Velocity (m/sec): | 0.05          |
| HALF-LIFE (hours) :       | 1.393 98.61   |
| HALF-LIFE (days ) :       | 0.05805 4.109 |

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility  
 =====

(using 10000 hr Bio P,A,S)  
 PROPERTIES OF: Ethane, 1,2-dichloro-

|  |                      |
|--|----------------------|
| Molecular weight (g/mol)   | 98.96                |
| Aqueous solubility (mg/l)  | 8600                 |
| Vapour pressure (Pa)   | 10519.1              |
| (atm)  | 0.103816             |
| (mm Hg)  | 78.9                 |
| Henry 's law constant (Atm-m <sup>3</sup> /mol)  | 0.00154              |
| Air-water partition coefficient  | 0.0629814            |
| Octanol-water partition coefficient (Kow)  | 30.1995              |
| Log Kow  | 1.48                 |
| Biomass to water partition coefficient   | 6.8399               |
| Temperature [deg C]  | 25                   |
| Biodeg rate constants (h <sup>-1</sup> ), half life in biomass (h) and in 2000 mg/L MLSS (h) : |                      |
| -Primary tank  | 0.01 134.95 10000.00 |
| -Aeration tank   | 0.01 134.95 10000.00 |
| -Settling tank   | 0.01 134.95 10000.00 |

STP Overall Chemical Mass Balance:  
 -----

| g/h            | mol/h     | percent         |
|----------------|-----------|-----------------|
| Influent       | 1.00E+001 | 1.0E-001 100.00 |
| Primary sludge | 3.18E-002 | 3.2E-004 0.32   |

|                         |           |          |       |
|-------------------------|-----------|----------|-------|
| Waste sludge            | 9.56E-002 | 9.7E-004 | 0.96  |
| Primary volatilization  | 1.14E-001 | 1.1E-003 | 1.14  |
| Settling volatilization | 1.93E-001 | 1.9E-003 | 1.93  |
| Aeration off gas        | 3.53E+000 | 3.6E-002 | 35.25 |
| Primary biodegradation  | 1.76E-003 | 1.8E-005 | 0.02  |
| Settling biodegradation | 3.28E-004 | 3.3E-006 | 0.00  |
| Aeration biodegradation | 4.39E-003 | 4.4E-005 | 0.04  |
| Final water effluent    | 6.03E+000 | 6.1E-002 | 60.35 |
| Total removal           | 3.97E+000 | 4.0E-002 | 39.65 |
| Total biodegradation    | 6.47E-003 | 6.5E-005 | 0.06  |

Level III Fugacity Model (Full-Output): User Koc

=====  
 Chem Name : Ethane, 1,2-dichloro-  
 Molecular Wt: 98.96  
 Henry's LC : 0.00154 atm-m3/mole (user-entered)  
 Vapor Press : 78.9 mm Hg (user-entered)  
 Log Kow : 1.48 (user-entered)  
 Soil Koc : 59 (user-entered)

| Mass Amount<br>(percent) | Half-Life<br>(hr) | Emissions<br>(kg/hr) |           |
|--------------------------|-------------------|----------------------|-----------|
| Air                      | 61.9              | 51                   | 9.09e+004 |
| Water                    | 5.93              | 8.76e+003            | 700       |
| Soil                     | 32.1              | 8.76e+003            | 8400      |
| Sediment                 | 0.0282            | 8.76e+003            | 0         |

| Fugacity<br>(atm) | Reaction<br>(kg/hr) | Advection<br>(kg/hr) | Reaction<br>(percent) | Advection<br>(percent) |           |
|-------------------|---------------------|----------------------|-----------------------|------------------------|-----------|
| Air               | 1.04e-008           | 5.73e+004            | 4.21e+004             | 57.3                   | 42.1      |
| Water             | 3.14e-008           | 31.9                 | 403                   | 0.0319                 | 0.403     |
| Soil              | 1.09e-006           | 173                  | 0                     | 0.173                  | 0         |
| Sediment          | 3.08e-008           | 0.152                | 0.0383                | 0.000152               | 3.83e-005 |

Persistence Time: 68 hr  
 Reaction Time: 118 hr  
 Advection Time: 160 hr  
 Percent Reacted: 57.5  
 Percent Advected: 42.5

Water Compartment Percents:

-----  

| Mass Amount<br>(percent) | Half-Life<br>(hr) | Emissions<br>(kg/hr) |           |
|--------------------------|-------------------|----------------------|-----------|
| Air                      | 61.9              | 51                   | 9.09e+004 |
| Water                    | 5.93              | 8.76e+003            | 700       |
| water                    | (5.93)            |                      |           |
| biota                    | (8.95e-006)       |                      |           |
| suspended sediment       | (0.000525)        |                      |           |
| Soil                     | 32.1              | 8.76e+003            | 8400      |
| Sediment                 | 0.0282            | 8.76e+003            | 0         |

Half-Lives (hr), (based upon user-entry):  
 Air: 51  
 Water: 8760  
 Soil: 8760

Sediment: 8760

Advection Times (hr):

Air: 100  
Water: 1000  
Sediment: 5e+004

Level III Fugacity Model (Full-Output): EQC Default

=====  
Chem Name : Ethane, 1,2-dichloro-  
Molecular Wt: 98.96  
Henry's LC : 0.00154 atm-m3/mole (user-entered)  
Vapor Press : 78.9 mm Hg (user-entered)  
Log Kow : 1.48 (user-entered)  
Soil Koc : 12.4 (EQC Model Default)

| Mass Amount<br>(percent) | Half-Life<br>(hr) | Emissions<br>(kg/hr) |           |
|--------------------------|-------------------|----------------------|-----------|
| Air 78.1                 |                   | 51                   | 9.09e+004 |
| Water 7.49               |                   | 8.76e+003            | 700       |
| Soil 14.4                |                   | 8.76e+003            | 8400      |
| Sediment 0.0188          |                   | 8.76e+003            | 0         |

| Fugacity<br>(atm)  | Reaction<br>(kg/hr) | Advection<br>(kg/hr) | Reaction<br>(percent) | Advection<br>(percent) |           |
|--------------------|---------------------|----------------------|-----------------------|------------------------|-----------|
| Air 1.04e-008      |                     | 5.73e+004            | 4.22e+004             | 57.3                   | 42.2      |
| Water 3.15e-008    |                     | 32                   | 405                   | 0.032                  | 0.405     |
| Soil 1.11e-006     |                     | 61.8                 | 0                     | 0.0618                 | 0         |
| Sediment 3.04e-008 |                     | 0.0803               | 0.0203                | 8.03e-005              | 2.03e-005 |

Persistence Time: 54 hr  
Reaction Time: 94.1 hr  
Advection Time: 127 hr  
Percent Reacted: 57.4  
Percent Advected: 42.6

Water Compartment Percents:

-----  
Mass Amount Half-Life Emissions  
(percent) (hr) (kg/hr)  
Air 78.1 51 9.09e+004  
Water 7.49 8.76e+003 700  
water (7.49)  
biota (1.13e-005)  
suspended sediment (0.000139)  
Soil 14.4 8.76e+003 8400  
Sediment 0.0188 8.76e+003 0

Half-Lives (hr), (based upon user-entry):

Air: 51  
Water: 8760  
Soil: 8760  
Sediment: 8760

Advection Times (hr):

Air: 100  
Water: 1000  
Sediment: 5e+004

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