United States
Environmental Protection Agency

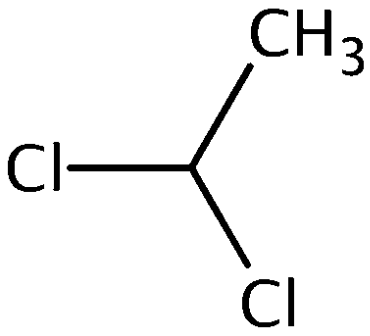
June 2025
Office of Chemical Safety and
Pollution Prevention

Risk Evaluation for 1,1-Dichloroethane

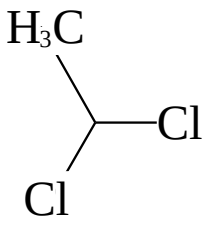
Supplemental Information File:

Supplemental Information on EPI Suite Modeling Results in the Fate Assessment

CASRN: 75-34-3



June 2025



```
SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
----------------------------- EPI SUMMARY (v4.11) -------------------------
Physical Property Inputs:
Log Kow (octanol-water):   1.79
Boiling Point (deg C)  :   57.40
Melting Point (deg C)  :   -96.90
Vapor Pressure (mm Hg) :   228
Water Solubility (mg/L):   5040
Henry LC (atm-m3/mole) :   0.00562


KOWWIN Program (v1.68) Results:
================================

Log Kow(version 1.68 estimate): 1.76

Experimental Database Structure Match:
Name     :  1,1-DICHLOROETHANE
CAS Num  :  000075-34-3
Exp Log P:  1.79
Exp Ref  :  HANSCH,C ET AL. (1995)

SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
-------+-----+-----------------------------------------+---------+--------
TYPE   | NUM |        LOGKOW FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
-------+-----+-----------------------------------------+---------+--------
Frag   |  1  |  -CH3    [aliphatic carbon]             | 0.5473  |  0.5473
Frag   |  1  |  -CH     [aliphatic carbon]             | 0.3614  |  0.3614
Frag   |  2  |  -CL     [chlorine, aliphatic attach]   | 0.3102  |  0.6204
Const  |     |  Equation Constant                      |         |  0.2290
-------+-----+-----------------------------------------+---------+--------
Log Kow   =   1.7581


MPBPVP (v1.43) Program Results:
================================
Experimental Database Structure Match:
Name     :  1,1-DICHLOROETHANE
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CAS Num  :  000075-34-3
Exp MP (deg C):  -96.9
Exp BP (deg C):  57.4
Exp VP (mm Hg):  2.27E+02
(Pa   ):  3.03E+004
Exp VP (deg C):  25
Exp VP ref    :  DAUBERT,TE & DANNER,RP (1985)

SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
------------------------ SUMMARY MPBVP v1.43 --------------------


Boiling Point:   63.01 deg C (Adapted Stein and Brown Method)

Melting Point: -116.02 deg C (Adapted Joback Method)
Melting Point:  -76.87 deg C (Gold and Ogle Method)
Mean Melt Pt :  -96.44 deg C (Joback; Gold,Ogle Methods)
Selected MP:  -96.44 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 57.40 deg C (user entered))
(MP not used for liquids)
VP:  222 mm Hg (Antoine Method)
:  2.95E+004 Pa  (Antoine Method)
VP:  216 mm Hg (Modified Grain Method)
:  2.87E+004 Pa  (Modified Grain Method)
VP:  240 mm Hg (Mackay Method)
:  3.2E+004 Pa  (Mackay Method)
Selected VP:  219 mm Hg (Mean of Antoine & Grain methods)
:  2.91E+004 Pa  (Mean of Antoine & Grain methods)



-------+-----+--------------------+----------+---------
TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
Group |  1  |  -CH3              |   21.98  |   21.98
Group |  1  |  >CH-              |   11.86  |   11.86
Group |  2  |  -Cl (secondary)   |   49.41  |   98.82
*   |     |  Equation Constant |          |  198.18
============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  330.84
RESULT- corr |  BOILING POINT in deg Kelvin  |  336.17
|  BOILING POINT in deg C       |   63.01
-----------------------------------------------------

-------+-----+--------------------+----------+---------
TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
Group |  1  |  -CH3              |   -5.10  |   -5.10
Group |  1  |  >CH-              |   12.64  |   12.64
Group |  2  |  -Cl (secondary)   |   13.55  |   27.10
*   |     |  Equation Constant |          |  122.50
============+====================+==========+=========
RESULT    |  MELTING POINT in deg Kelvin  |  157.14
|  MELTING POINT in deg C       | -116.02
-----------------------------------------------------
```

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

Water Sol: 4564 mg/L

Experimental Water Solubility Database Match:
Name     :  1,1-DICHLOROETHANE
CAS Num  :  000075-34-3
Exp WSol :  5040 mg/L (25 deg C)
Exp Ref  :  HORVATH,AL ET AL. (1999)

SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
---------------------------------- WSKOW v1.42 Results -----------------------
Log Kow  (estimated)  :  1.76
Log Kow (experimental):  1.79
Cas No: 000075-34-3
Name  : 1,1-DICHLOROETHANE
Refer : HANSCH,C ET AL. (1995)
Log Kow used by Water solubility estimates:  1.79 (user entered)

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

Melting Pt (Tm) = -96.90 deg C (Use Tm = 25 for all liquids)

Correction(s):         Value
--------------------   -----
No Applicable Correction Factors

Log Water Solubility  (in moles/L) :  -1.336
Water Solubility at 25 deg C (mg/L):  4564



WATERNT Program (v1.01) Results:
================================

Water Sol (v1.01 est): 6614.3 mg/L

Experimental Water Solubility Database Match:
Name     :  1,1-DICHLOROETHANE
CAS Num  :  000075-34-3
Exp WSol :  5040 mg/L (25 deg C)
Exp Ref  :  HORVATH,AL ET AL. (1999)

SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
-------+-----+---------------------------------------------+----------+---------
TYPE   | NUM |    WATER SOLUBILITY FRAGMENT DESCRIPTION    |  COEFF   |  VALUE
-------+-----+---------------------------------------------+----------+---------
Frag   |  1  |  -CH3    [aliphatic carbon]                 |-0.3213   | -0.3213
Frag   |  1  |  -CH     [aliphatic carbon]                 |-0.5285   | -0.5285
Frag   |  2  |  -CL     [chlorine, aliphatic attach]       |-0.2872   | -0.5744
Const  |     |  Equation Constant                          |          |  0.2492
-------+-----+---------------------------------------------+----------+---------
```

Log Water Sol (moles/L) at 25 dec C =   -1.1750
Water Solubility (mg/L) at 25 dec C =   6614.3

ECOSAR Program (v1.11) Results:
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ECOSAR Version 1.11 Results Page

SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
CAS Num:
ChemID1:
MOL FOR: C2 H4 CL2
MOL WT : 98.96
Log Kow: 1.758   (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: 1.79   (PhysProp DB exp value - for comparison only)
Melt Pt: -96.90   (deg C, User Entered for Wat Sol estimate)
Melt Pt: -96.90   (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 4564   (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: 5040   (mg/L, User Entered)
Wat Sol: 5040   (mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 1.758   (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 5040   (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	134.064
Neutral Organics	Daphnid	48-hr	LC50	74.441
Neutral Organics	Green Algae	96-hr	EC50	50.560
Neutral Organics	Fish		ChV	12.763
Neutral Organics	Daphnid		ChV	6.822
Neutral Organics	Green Algae		ChV	12.598
Neutral Organics	Fish (SW)	96-hr	LC50	168.532
Neutral Organics	Mysid	96-hr	LC50	147.553
Neutral Organics	Fish (SW)		ChV	15.781
Neutral Organics	Mysid (SW)		ChV	13.702
Neutral Organics	Earthworm	14-day	LC50	182.283

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

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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:  4.77E-003 atm-m3/mole  (4.83E+002 Pa-m3/mole)

SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
--------------------------- HENRYWIN v3.20 Results -------------------------

Experimental Database Structure Match:
Name     :  1,1-DICHLOROETHANE
CAS Num  :  000075-34-3
Exp HLC  :  5.62E-03 atm-m3/mole  (569 Pa-m3/mole)
Temper   :  24 deg C
Exp Ref  :  GOSSETT,JM (1987)

----------+-----------------------------------------------+---------+----------
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
--------+-----------------------------------------------+-----------+--------
|           1  CH3 (X)                          |            | -0.62
|           1  CH (C)(CL)(CL)                   |            |  1.33
--------+-----------------------------------------------+-----------+--------
RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |    TOTAL   |  0.71
--------+-----------------------------------------------+-----------+--------
HENRYs LAW CONSTANT at 25 deg C = 4.77E-003 atm-m3/mole
= 1.95E-001 unitless
= 4.83E+002 Pa-m3/mole


For Henry LC Comparison Purposes:
Exper Database: 5.62E-03  atm-m3/mole  (5.69E+002 Pa-m3/mole)
User-Entered Henry LC:  5.620E-003 atm-m3/mole  (5.694E+002 Pa-m3/mole)
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Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC:  5.890E-003 atm-m3/mole  (5.969E+002 Pa-m3/mole)
VP:   228 mm Hg (source: User-Entered)
WS:   5.04E+003 mg/L (source: User-Entered)


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

Log Koa: 2.429

SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
--------------------------- KOAWIN v1.10 Results --------------------------

Experimental Database Structure Match:
Name      :  1,1-Dichloroethane
CAS Num   :  000075-34-3
Exp LogKoa:  2.41
Exp Ref   :  Abraham,MH et al. (2001)

Log Koa (octanol/air) estimate:  2.429
Koa (octanol/air) estimate:  268.4
Using:
Log Kow:  1.79  (user entered)
HenryLC:  0.00562  atm-m3/mole (user entered)
Log Kaw:  -0.639  (air/water part.coef.)

LogKow  : 1.79 (exp database)
LogKow  : 1.76 (KowWin estimate)
Henry LC: 0.00562 atm-m3/mole (exp database)
Henry LC: 0.0121 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate:  2.066 (from KowWin/HenryWin)


BIOWIN (v4.10) Program Results:
===============================
SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
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]	0.0011	0.0022
Frag	1	Methyl [-CH3]	0.0004	0.0004
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-0.2944
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.3696

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aliphatic chloride [-CL]	-0.6391	-1.2783
Frag	1	Methyl [-CH3]	0.0194	0.0194
Frag	1	-CH- [linear]	-0.0998	-0.0998
MolWt	*	Molecular Weight Parameter		-2.8569

```
RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.1558
============+============================================+=========+=========

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 |  1  |  Methyl  [-CH3]                            | -0.0796 | -0.0796
Frag |  1  |  -CH-   [linear]                           | -0.1659 | -0.1659
Const|  *  |  Equation Constant                         |         |  0.8361
============+============================================+=========+=========
RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)   |         |  0.5613
============+============================================+=========+=========

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 >= 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 (CERIJ) database.

BioHCwin (v1.01) Program Results:
================================
SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
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):  3.04E+004 Pa (228 mm Hg)
Log Koa (Exp database): 2.410
Kp (particle/gas partition coef. (m3/ug)):
Mackay model           :  9.87E-011
Octanol/air (Koa) model:  6.31E-011
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model     :  3.56E-009
Mackay model           :  7.89E-009
Octanol/air (Koa) model:  5.05E-009


AOP Program (v1.92) Results:
```

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==========================
SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
------------------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction       =   0.3291 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 =   0.3291 E-12 cm3/molecule-sec
HALF-LIFE =    32.501 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 :  1,1-Dichloroethane
CAS Number:  000075-34-3
Exper OH rate constant   :  0.274  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):
5.73E-009 (Junge-Pankow, Mackay avg)
5.05E-009 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation



KOCWIN Program (v2.00) Results:
==============================
SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96

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Experimental Database Structure Match:
Name     :  1,1-DICHLOROETHANE
CAS Num  :  000075-34-3
Exp LogKoc:  1.48
Exp Ref  :  Sabljic,A et al (1995)

---------------------------  KOCWIN v2.00 Results  --------------------------

Koc Estimate from MCI:
----------------------
First Order Molecular Connectivity Index  ..........  :  1.732
Non-Corrected Log Koc (0.5213 MCI + 0.60)  ..........  :  1.5027
Fragment Correction(s) -->  NONE                       :   ---
Corrected Log Koc  ................................... :  1.5027

Estimated Koc:  31.82  L/kg   <===========

Koc Estimate from Log Kow:
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```
-------------------------
Log Kow  (User entered   )  ......................... :  1.79
Non-Corrected Log Koc (0.8679 logKow - 0.0004)  ..... :  1.5531
Fragment Correction(s) -->  NONE                      :   ---
Corrected Log Koc  ................................. :  1.5531

Estimated Koc:  35.74  L/kg   <==========


HYDROWIN Program (v2.00) Results:
================================
SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
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: -CH-CL2
|              R2: -H
R3             R3: -H
Kb hydrolysis at atom #  4:  9.158E-010  L/mol-sec

Total Kb for pH > 8 at 25 deg C :  9.158E-010  L/mol-sec
Kb Half-Life at pH 8: 2.398E+007  years
Kb Half-Life at pH 7: 2.398E+008  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!



BCFBAF Program (v3.01) Results:
==============================
SMILES : C(CL)(CL)C
CHEM   : 1,1-DICHLOROETHANE
MOL FOR: C2 H4 CL2
MOL WT : 98.96
-------------------------------- BCFBAF v3.01 --------------------------------
Summary Results:
Log BCF (regression-based estimate):  0.85  (BCF = 7.05 L/kg wet-wt)
Biotransformation Half-Life (days) :  0.343  (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic):  0.83  (BAF = 6.79 L/kg wet-wt)

Log Kow (experimental):  1.79
Log Kow used by BCF estimates:  1.79 (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 =  0.848  (BCF = 7.048 L/kg wet-wt)
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============================================================
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 |  1  |  Methyl  [-CH3]                           |  0.2451 |  0.2451
Frag |  1  |  -CH-   [linear]                          | -0.1912 | -0.1912
L Kow|  *  |  Log Kow =   1.79 (user-entered   )       |  0.3073 |  0.5501
MolWt|  *  |  Molecular Weight Parameter               |         | -0.2538
Const|  *  |  Equation Constant                        |         | -1.5371
============+=========================================+=========+=========
RESULT   |        LOG Bio Half-Life (days)           |         | -0.4653
RESULT   |            Bio Half-Life (days)           |         |  0.3425
NOTE     |  Bio Half-Life Normalized to 10 g fish at 15 deg C   |
============+=========================================+=========+=========

Biotransformation Rate Constant:
kM (Rate Constant):  2.024 /day (10 gram fish)
kM (Rate Constant):  1.138 /day (100 gram fish)
kM (Rate Constant):  0.6399 /day (1 kg fish)
kM (Rate Constant):  0.3599 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) =  0.832  (BCF = 6.791 L/kg wet-wt)
Estimated Log BAF (upper trophic) =  0.832  (BAF = 6.791 L/kg wet-wt)
Estimated Log BCF (mid trophic)   =  0.693  (BCF = 4.934 L/kg wet-wt)
Estimated Log BAF (mid trophic)   =  0.693  (BAF = 4.934 L/kg wet-wt)
Estimated Log BCF (lower trophic) =  0.651  (BCF = 4.473 L/kg wet-wt)
Estimated Log BAF (lower trophic) =  0.651  (BAF = 4.474 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) =  0.874  (BCF = 7.487 L/kg wet-wt)
Estimated Log BAF (upper trophic) =  0.882  (BAF = 7.622 L/kg wet-wt)



Volatilization From Water
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Chemical Name: 1,1-DICHLOROETHANE

Molecular Weight    :  98.96 g/mole
Water Solubility    :  5040 ppm
Vapor Pressure      :  228 mm Hg
Henry's Law Constant:  0.00562 atm-m3/mole  (entered by user)

RIVER             LAKE
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Water Depth     (meters):   1                 1
Wind Velocity    (m/sec):   5                 0.5
Current Velocity (m/sec):   1                 0.05

HALF-LIFE (hours) :   1.119             95.62
HALF-LIFE (days ) :   0.04661           3.984


STP Fugacity Model:  Predicted Fate in a Wastewater Treatment Facility
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(using 10000 hr Bio P,A,S)
PROPERTIES OF: 1,1-DICHLOROETHANE

Molecular weight (g/mol)		98.96
Aqueous solubility (mg/l)		5040
Vapour pressure (Pa)		30397.5
(atm)	0.3	
(mm Hg)	228	
Henry 's law constant (Atm-m3/mol)		0.00562
Air-water partition coefficient		0.229841
Octanol-water partition coefficient (Kow)		61.6595
Log Kow		1.79
Biomass to water partition coefficient		13.1319
Temperature [deg C]		25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	255.92	10000.00
-Aeration tank	0.00	255.92	10000.00
-Settling tank	0.00	255.92	10000.00

STP Overall Chemical Mass Balance:

g/h	mol/h	percent	
Influent	1.00E+001	1.0E-001	100.00
Primary sludge	3.91E-002	4.0E-004	0.39
Waste sludge	5.05E-002	5.1E-004	0.50
Primary volatilization	1.26E-001	1.3E-003	1.26
Settling volatilization	1.09E-001	1.1E-003	1.09
Aeration off gas	6.59E+000	6.7E-002	65.86
Primary biodegradation	1.77E-003	1.8E-005	0.02
Settling biodegradation	1.70E-004	1.7E-006	0.00
Aeration biodegradation	2.27E-003	2.3E-005	0.02
Final water effluent	3.09E+000	3.1E-002	30.85
Total removal	6.91E+000	7.0E-002	69.15
Total biodegradation	4.22E-003	4.3E-005	0.04

Level III Fugacity Model (Full-Output):

Chem Name : 1,1-DICHLOROETHANE
Molecular Wt: 98.96
Henry's LC : 0.00562 atm-m3/mole (user-entered)
Vapor Press : 228 mm Hg (user-entered)
Log Kow : 1.79 (user-entered)
Soil Koc : 31.8 (KOCWIN MCI method)

Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air 84.8	936	1.81
Water 15.1	2.76e+003	0.11
Soil 0.0761	2.76e+003	0.000114
Sediment 0.0466	2.76e+003	0

Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)	
Air	4.32e-013	0.13	1.75	6.75	91.2

Water	8.85e-012	0.00783	0.0312	0.408	1.62
Soil	4.47e-013	3.95e-005	0	0.00206	0
Sediment	7.74e-012	2.42e-005	1.92e-006	0.00126	0.0001

Persistence Time: 108 hr
Reaction Time: 1.5e+003 hr
Advection Time: 116 hr
Percent Reacted: 7.16
Percent Advected: 92.8

Half-Lives (hr), (based upon user-entry):
Air: 936
Water: 2760
Soil: 2760
Sediment: 2760

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

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