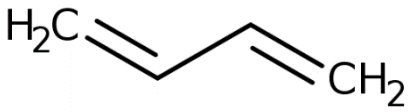
United States
Environmental Protection Agency

November 2024
Office of Chemical Safety and
Pollution Prevention

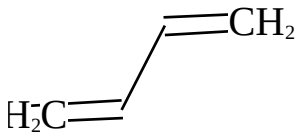
Draft EPI Suite Modeling Results Supporting Fate Assessment for 1,3-Butadiene

CASRN: 106-99-0



November 2024

EPI Suite Results For CAS 000106-99-0



```
SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
------------------------------ EPI SUMMARY (v4.11) -------------------------
Physical Property Inputs:
Log Kow (octanol-water):   1.99
Boiling Point (deg C)  :   -4.54
Melting Point (deg C)  :   -109.00
Vapor Pressure (mm Hg) :   1900
Water Solubility (mg/L):   735
Henry LC (atm-m3/mole) :   0.076

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

Log Kow(version 1.69 estimate): 2.03

Experimental Database Structure Match:
Name     :  1,3-BUTADIENE
CAS Num  :  000106-99-0
Exp Log P:  1.99
Exp Ref  :  HANSCH,C ET AL. (1995)

SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
-------+-----+-----------------------------------------+---------+--------
TYPE   | NUM |        LOGKOW FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
-------+-----+-----------------------------------------+---------+--------
Frag   |  2  |  =CH2    [olefinic carbon]              | 0.5184  |  1.0368
Frag   |  2  |  =CH- or =C<  [olefinc carbon]          | 0.3836  |  0.7672
Const  |     |  Equation Constant                      |         |  0.2290
-------+-----+-----------------------------------------+---------+--------
Log Kow    =   2.0330
```

```
MPBPVP (v1.43) Program Results:
===============================
Experimental Database Structure Match:
Name     :  1,3-BUTADIENE
CAS Num  :  000106-99-0
Exp MP (deg C):  -108.9
Exp BP (deg C):  -4.4
Exp VP (mm Hg):  2.11E+03
(Pa   ):  2.81E+005
Exp VP (deg C):  25
Exp VP ref    :  DAUBERT,TE & DANNER,RP (1985)

SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
------------------------ SUMMARY MPBPWIN v1.44 --------------------


Boiling Point:   15.55 deg C (Adapted Stein and Brown Method)

Melting Point: -141.84 deg C (Adapted Joback Method)
Melting Point: -104.58 deg C (Gold and Ogle Method)
Mean Melt Pt : -123.21 deg C (Joback; Gold,Ogle Methods)
Selected MP: -123.21 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: -4.54 deg C (user entered))
(MP not used for liquids)
VP:  2.1E+003 mm Hg (Antoine Method)
:  2.8E+005 Pa  (Antoine Method)
VP:  2.03E+003 mm Hg (Modified Grain Method)
:  2.7E+005 Pa  (Modified Grain Method)
VP:  1.96E+003 mm Hg (Mackay Method)
:  2.61E+005 Pa  (Mackay Method)
Selected VP:  2.06E+003 mm Hg (Mean of Antoine & Grain methods)
:  2.75E+005 Pa  (Mean of Antoine & Grain methods)



-------+-----+--------------------+----------+---------
TYPE   | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
Group |  2   |  =CH2              |   16.44  |   32.88
Group |  2   |  =CH-              |   27.95  |   55.90
*     |      |  Equation Constant |          |  198.18
============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin  |  286.96
RESULT- corr |  BOILING POINT in deg Kelvin  |  288.71
|  BOILING POINT in deg C       |   15.55
-----------------------------------------------------

-------+-----+--------------------+----------+---------
TYPE   | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
```

```
-------+-----+--------------------+----------+---------
Group |  2  |  =CH2              |   -4.32  |   -8.64
Group |  2  |  =CH-              |    8.73  |   17.46
*   |     |  Equation Constant |          |  122.50
============+====================+==========+=========
RESULT    |  MELTING POINT in deg Kelvin  |  131.32
|  MELTING POINT in deg C       | -141.84
-----------------------------------------------------
```

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

Water Sol: 803.3 mg/L

Experimental Water Solubility Database Match:
Name     :  1,3-BUTADIENE
CAS Num  :  000106-99-0
Exp WSol :  735 mg/L (25 deg C)
Exp Ref  :  MCAULIFFE,C (1966)

SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
---------------------------------- WSKOW v1.43 Results ------------------------
Log Kow  (estimated)  :  2.03
Log Kow (experimental):  1.99
Cas No: 000106-99-0
Name  : 1,3-BUTADIENE
Refer : HANSCH,C ET AL. (1995)
Log Kow used by Water solubility estimates:  1.99 (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) = -109.00 deg C (Use Tm = 25 for all liquids)

Correction(s):         Value
--------------------   -----
Hydrocarbon          -0.441

Log Water Solubility  (in moles/L) :  -1.828
Water Solubility at 25 deg C (mg/L):  803.3


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

Water Sol (v1.01 est): 1974.2 mg/L

Experimental Water Solubility Database Match:
Name     :  1,3-BUTADIENE
CAS Num  :  000106-99-0
Exp WSol :  735 mg/L (25 deg C)
```

Exp Ref : MCAULIFFE,C (1966)

SMILES : C(C=C)=C
CHEM : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	=CH2 [olefinic carbon]	-0.4789	-0.9578
Frag	2	=CH- or =C< [olefinc carbon]	-0.3646	-0.7292
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -1.4377
Water Solubility (mg/L) at 25 dec C = 1974.2

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

SMILES : C(C=C)=C
CHEM : 1,3-BUTADIENE
CAS Num:
ChemID1:
MOL FOR: C4 H6
MOL WT : 54.09
Log Kow: 2.033 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Log Kow: 1.99 (PhysProp DB exp value - for comparison only)
Melt Pt: -109.00 (deg C, User Entered for Wat Sol estimate)
Melt Pt: -108.90 (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 803.3 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wat Sol: 735 (mg/L, User Entered)
Wat Sol: 735 (mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 2.033 (EPISuite Kowwin v1.68 Estimate)
Wat Sol: 735 (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	41.505
Neutral Organics	: Daphnid	48-hr	LC50	23.639
Neutral Organics	: Green Algae	96-hr	EC50	17.832
Neutral Organics	: Fish		ChV	4.072

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Neutral Organics          : Daphnid                      ChV         2.325
Neutral Organics          : Green Algae                  ChV         4.702
Neutral Organics          : Fish (SW)          96-hr     LC50       52.262
Neutral Organics          : Mysid              96-hr     LC50       37.982
Neutral Organics          : Fish (SW)                    ChV         5.788
Neutral Organics          : Mysid (SW)                   ChV         3.251
Neutral Organics          : Earthworm          14-day    LC50       93.307

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.


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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:
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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 :  7.79E-002 atm-m3/mole  (7.90E+003 Pa-m3/mole)
Group Est:  7.05E-002 atm-m3/mole  (7.15E+003 Pa-m3/mole)

SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
--------------------------- HENRYWIN v3.21 Results -------------------------

Experimental Database Structure Match:
Name     :  1,3-BUTADIENE
CAS Num  :  000106-99-0
Exp HLC  :  7.36E-02 atm-m3/mole  (7.46E+003 Pa-m3/mole)
Temper   :  25 deg C
Exp Ref  :  VP/WSOL

----------+-----------------------------------------------+---------+----------
CLASS  |     BOND CONTRIBUTION DESCRIPTION           | COMMENT |  VALUE
----------+-----------------------------------------------+---------+----------
HYDROGEN |   6  Hydrogen to Carbon (olefinic) Bonds    |         | -0.6029
FRAGMENT |   1  Cd-Cd                                  |         |  0.0997
FRAGMENT |   2  Cd=Cd                                  |         |  0.0000
----------+-----------------------------------------------+---------+----------
```

```
RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE    |  TOTAL  | -0.503
---------+-----------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 7.79E-002 atm-m3/mole
= 3.19E+000 unitless
= 7.90E+003 Pa-m3/mole

--------+-----------------------------------------------+------------+--------
|        GROUP CONTRIBUTION DESCRIPTION         |   COMMENT  |  VALUE
--------+-----------------------------------------------+------------+--------
|           2  Cd-H2                            |            | -0.82
|           2  CdH (Cd)                         |            |  0.36
--------+-----------------------------------------------+------------+--------
RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |    TOTAL   | -0.46
--------+-----------------------------------------------+------------+--------
HENRYs LAW CONSTANT at 25 deg C = 7.05E-002 atm-m3/mole
= 2.88E+000 unitless
= 7.15E+003 Pa-m3/mole


For Henry LC Comparison Purposes:
Exper Database: 7.36E-02  atm-m3/mole  (7.46E+003 Pa-m3/mole)
User-Entered Henry LC:  7.600E-002 atm-m3/mole  (7.701E+003 Pa-m3/mole)
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC:  7.359E-002 atm-m3/mole  (7.457E+003 Pa-m3/mole)
VP:   1.9E+003 mm Hg (source: User-Entered)
WS:   735 mg/L (source: User-Entered)



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

Log Koa: 1.498

SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
--------------------------- KOAWIN v1.10 Results --------------------------

Log Koa (octanol/air) estimate:  1.498
Koa (octanol/air) estimate:  31.45
Using:
Log Kow:  1.99  (user entered)
HenryLC:  0.076  atm-m3/mole (user entered)
Log Kaw:  0.492  (air/water part.coef.)

LogKow  : 1.99 (exp database)
LogKow  : 2.03 (KowWin estimate)
Henry LC: 0.0736 atm-m3/mole (exp database)
Henry LC: 0.0779 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate:  1.527 (from KowWin/HenryWin)



BIOWIN (v4.10) Program Results:
```

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==============================
SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
--------------------------- BIOWIN v4.10 Results ---------------------------

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

------+-----+-------------------------------------------+---------+---------
TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION         |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
MolWt|  *  |  Molecular Weight Parameter                |         | -0.0258
Const|  *  |  Equation Constant                         |         |  0.7475
============+===========================================+=========+=========
RESULT   |    Biowin1 (Linear Biodeg Probability)      |         |  0.7218
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION         |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
MolWt|  *  |  Molecular Weight Parameter                |         | -0.7681
============+===========================================+=========+=========
RESULT   |  Biowin2 (Non-Linear Biodeg Probability)    |         |  0.9038
============+===========================================+=========+=========

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
------+-----+-------------------------------------------+---------+---------
MolWt|  *  |  Molecular Weight Parameter                |         | -0.1195
Const|  *  |  Equation Constant                         |         |  3.1992
============+===========================================+=========+=========
RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)   |         |  3.0796
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION         |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
MolWt|  *  |  Molecular Weight Parameter                |         | -0.0780
Const|  *  |  Equation Constant                         |         |  3.8477
============+===========================================+=========+=========
RESULT   |   Biowin4 (Survey Model - Primary Biodeg)   |         |  3.7697
============+===========================================+=========+=========

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	6	-C=CH [alkenyl hydrogen]	-0.0058	-0.0350
MolWt	*	Molecular Weight Parameter		-0.0853
Const	*	Equation Constant		0.5544
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.4341

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	-C=CH [alkenyl hydrogen]	-0.0921	-0.5528
MolWt	*	Molecular Weight Parameter		-0.9358
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.5433

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	6	-C=CH [alkenyl hydrogen]	-0.0735	-0.4411
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.3949

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(C=C)=C
CHEM : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
---------- BioHCwin v1.01 Results ----------

TYPE	NUM	LOG Hydrocarbon FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	-C=CH [alkenyl hydrogen]	-0.0066	-0.0398
Const	*	Equation Constant		0.4898
RESULT		LOG BioHC Half-Life (days)		0.4499
RESULT		BioHC Half-Life (days)		2.818

```
AEROWIN Program (v1.00) Results:
================================
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled):  2.53E+005 Pa (1.9E+003 mm Hg)
Log Koa (Koawin est  ): 1.498
Kp (particle/gas partition coef. (m3/ug)):
Mackay model           :  1.18E-011
Octanol/air (Koa) model:  7.73E-012
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model     :  4.28E-010
Mackay model           :  9.47E-010
Octanol/air (Koa) model:  6.18E-010


AOP Program (v1.92) Results:
============================
SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
------------------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction       =   0.0000 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 =  66.6000 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 =  66.6000 E-12 cm3/molecule-sec
HALF-LIFE =     0.161 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE =     1.927 Hrs
------------------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----------
OVERALL OZONE Rate Constant =     0.810000 E-17 cm3/molecule-sec
HALF-LIFE =      1.415 Days (at 7E11 mol/cm3)
HALF-LIFE =     33.956 Hrs

Experimental Database Structure Match:
Chem Name :  1,3-BUTADIENE
CAS Number:  000106-99-0
Exper OH rate constant   :  69.3  E-12  cm3/molecule-sec
Exper OH Reference:  NIST Webbook
Exper Ozone rate constant:  6.23 E-18  cm3/molecule-sec
Exper NO3 rate constant  :  1.0 E-13  cm3/molecule-sec
```

```
Fraction sorbed to airborne particulates (phi):
6.88E-010 (Junge-Pankow, Mackay avg)
6.18E-010 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation



KOCWIN Program (v2.00) Results:
==============================
SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
--------------------------  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   )  ........................  :  1.99
Non-Corrected Log Koc (0.8679 logKow - 0.0004)  .....  :  1.7267
Fragment Correction(s) -->  NONE                      :   ---
Corrected Log Koc  ................................   :  1.7267

Estimated Koc:  53.3  L/kg   <==========



HYDROWIN Program (v2.00) Results:
=================================
SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
-------------------------- HYDROWIN v2.00 Results --------------------------


Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens),
Specific Alkyl Halides & Phosphorus Esters can be estimated!!

When present, various hydrolyzable compound-types will be identified.
For more information, (Click OVERVIEW in Help  or  see the User's Guide)

*****   CALCULATION NOT PERFORMED   *****
```

```
BCFBAF Program (v3.01) Results:
==============================
SMILES : C(C=C)=C
CHEM   : 1,3-BUTADIENE
MOL FOR: C4 H6
MOL WT : 54.09
--------------------------------- BCFBAF v3.01 ---------------------------------
Summary Results:
Log BCF (regression-based estimate):  0.98  (BCF = 9.55 L/kg wet-wt)
Biotransformation Half-Life (days) :  0.338  (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic):  1.00  (BAF = 10 L/kg wet-wt)

Log Kow (experimental):  1.99
Log Kow used by BCF estimates:  1.99 (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 =  0.980  (BCF = 9.55 L/kg wet-wt)

============================================================
Whole Body Primary Biotransformation Rate Estimate for Fish:
============================================================
------+-----+-------------------------------------------+---------+---------
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
Frag |  6  |  -C=CH  [alkenyl hydrogen]                 |  0.0988 |  0.5931
Frag |  6  |  -C=CH  [alkenyl hydrogen]                 |  0.0000 |  0.0000
L Kow|  *  |  Log Kow =   1.99 (user-entered   )        |  0.3073 |  0.6116
MolWt|  *  |  Molecular Weight Parameter                |         | -0.1387
Const|  *  |  Equation Constant                         |         | -1.5371
============+===========================================+=========+=========
RESULT   |        LOG Bio Half-Life (days)            |         | -0.4711
RESULT   |            Bio Half-Life (days)            |         |   0.338
NOTE     |  Bio Half-Life Normalized to 10 g fish at 15 deg C   |
============+===========================================+=========+=========

Biotransformation Rate Constant:
kM (Rate Constant):  2.051 /day (10 gram fish)
kM (Rate Constant):  1.153 /day (100 gram fish)
kM (Rate Constant):  0.6485 /day (1 kg fish)
kM (Rate Constant):  0.3647 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) =  1.000  (BCF = 10.01 L/kg wet-wt)
Estimated Log BAF (upper trophic) =  1.000  (BAF = 10.01 L/kg wet-wt)
Estimated Log BCF (mid trophic)   =  0.857  (BCF = 7.197 L/kg wet-wt)
Estimated Log BAF (mid trophic)   =  0.857  (BAF = 7.197 L/kg wet-wt)
Estimated Log BCF (lower trophic) =  0.812  (BCF = 6.484 L/kg wet-wt)
Estimated Log BAF (lower trophic) =  0.812  (BAF = 6.486 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
```

```
Estimated Log BCF (upper trophic) =  1.055  (BCF = 11.34 L/kg wet-wt)
Estimated Log BAF (upper trophic) =  1.065  (BAF = 11.6 L/kg wet-wt)
```

```
Volatilization From Water
=========================

Chemical Name: 1,3-BUTADIENE

Molecular Weight    :  54.09 g/mole
Water Solubility    :  735 ppm
Vapor Pressure      :  1900 mm Hg
Henry's Law Constant:  0.076 atm-m3/mole  (entered by user)

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

HALF-LIFE (min  ) :   45.37            4195
HALF-LIFE (hours) :   0.7562           69.92
HALF-LIFE (days ) :   0.03151          2.913
```

```
STP Fugacity Model:  Predicted Fate in a Wastewater Treatment Facility
=======================================================================
(using 10000 hr Bio P,A,S)
PROPERTIES OF: 1,3-BUTADIENE
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Molecular weight (g/mol)                              54.09
Aqueous solubility (mg/l)                             735
Vapour pressure (Pa)                                  253313
(atm)                                  2.5
(mm Hg)                                1900
Henry 's law constant (Atm-m3/mol)                    0.076
Air-water partition coefficient                       3.10817
Octanol-water partition coefficient (Kow)             97.7237
Log Kow                                               1.99
Biomass to water partition coefficient                20.3447
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       390.99       10000.00
-Aeration tank       0.00       390.99       10000.00
-Settling tank       0.00       390.99       10000.00

STP Overall Chemical Mass Balance:
----------------------------------
g/h               mol/h          percent

Influent                    1.00E+001         1.8E-001        100.00

Primary sludge              4.76E-002         8.8E-004         0.48
Waste sludge                5.57E-003         1.0E-004         0.06
```

Primary volatilization	1.31E-001	2.4E-003	1.31
Settling volatilization	1.21E-002	2.2E-004	0.12
Aeration off gas	9.47E+000	1.8E-001	94.74
Primary biodegradation	1.80E-003	3.3E-005	0.02
Settling biodegradation	1.83E-005	3.4E-007	0.00
Aeration biodegradation	2.45E-004	4.5E-006	0.00
Final water effluent	3.28E-001	6.1E-003	3.28
Total removal	9.67E+000	1.8E-001	96.72
Total biodegradation	2.06E-003	3.8E-005	0.02

(** Total removal recommended maximum is 95 percent)

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

Chem Name : 1,3-BUTADIENE
Molecular Wt: 54.09
Henry's LC : 0.076 atm-m3/mole (user-entered)
Vapor Press : 1.9e+003 mm Hg (user-entered)
Log Kow : 1.99 (user-entered)
Soil Koc : 53.7 (user-entered)

Mass Amount (percent)		Half-Life (hr)	Emissions (kg/hr)	
Air	0	5.09e-313	1000	
Water	95.9	360	1000	
Soil	3.68	720	1000	
Sediment	0.388	3.24e+003	0	

Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)	
Air	0	-1.#J	0	-1.#J	-1.#J
Water	1.3e-006	356	185	-1.#J	-1.#J
Soil	2.5e-007	6.81	0	-1.#J	-1.#J
Sediment	1.15e-006	0.16	0.0149	-1.#J	-1.#J

Persistence Time: 64.2 hr
Reaction Time: -1.#J hr
Advection Time: 1.04e+003 hr
Percent Reacted: -1.#J
Percent Advected: -1.#J

Water Compartment Percents:

Mass Amount (percent)		Half-Life (hr)	Emissions (kg/hr)	
Air	0	5.09e-313	1000	
Water	95.9	360	1000	
water	(95.9)			
biota	(0.000469)			
suspended sediment	(0.00773)			
Soil	3.68	720	1000	
Sediment	0.388	3.24e+003	0	

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

```
Air:      5.093e-313
Water:    360
Soil:     720
Sediment: 3240

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


Level III Fugacity Model (Full-Output): EQC Default
=====================================================
Chem Name   : 1,3-BUTADIENE
Molecular Wt: 54.09
Henry's LC  : 0.076 atm-m3/mole (user-entered)
Vapor Press : 1.9e+003 mm Hg  (user-entered)
Log Kow     : 1.99  (user-entered)
Soil Koc    : 40.1  (EQC Model Default)

Mass Amount    Half-Life    Emissions
(percent)        (hr)       (kg/hr)
Air       0               5.09e-313    1000
Water     96.5            360          1000
Soil      3.15            720          1000
Sediment  0.337           3.24e+003    0

Fugacity    Reaction    Advection   Reaction    Advection
(atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
Air       0            -1.#J       0           -1.#J       -1.#J
Water     1.3e-006     356         185         -1.#J       -1.#J
Soil      2.5e-007     5.81        0           -1.#J       -1.#J
Sediment  1.15e-006    0.138       0.0129      -1.#J       -1.#J

Persistence Time: 63.8 hr
Reaction Time:    -1.#J hr
Advection Time:   1.04e+003 hr
Percent Reacted:  -1.#J
Percent Advected: -1.#J

Water Compartment Percents:
---------------------------
Mass Amount    Half-Life    Emissions
(percent)        (hr)       (kg/hr)
Air       0               5.09e-313    1000
Water     96.5            360          1000
water     (96.5)
biota     (0.000472)
suspended sediment (0.0058)
Soil      3.15            720          1000
Sediment  0.337           3.24e+003    0

Half-Lives (hr), (based upon user-entry):
Air:      5.093e-313
Water:    360
Soil:     720
Sediment: 3240
```

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

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