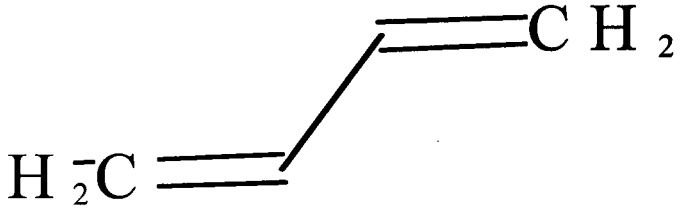

SMILES : C(C=C)=C
CHEM : 1,3-Butadiene
CAS NUM: 000106-99-0
MOL FOR: C4 H6
MOL WT : 54.09

---------- EPI SUMMARY (v3.12) ----------

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

KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 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

MPBPWIN (v1.41) 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
- 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 v1.41 ----------

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: -4.40 deg C (exp database))
  (MP not used for liquids)
    VP: 2.09E+003 mm Hg (Antoine Method)
    VP: 2.02E+003 mm Hg (Modified Grain Method)
    VP: 1.95E+003 mm Hg (Mackay Method)
  Selected VP: 2.05E+003 mm Hg (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 v1.41) Results:
==========

Water Sol: 792.3 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 v1.41 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

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
       (used when Melting Point NOT available)

Correction(s):	Value
Hydrocarbon	-0.537

   Log Water Solubility (in moles/L) : -1.834

Water Solubility at 25 deg C (mg/L): 792.3

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 (v0.99h) Results:
==========
SMILES : C(C=C)=C
CHEM : 1,3-Butadiene
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C4 H6
MOL WT : 54.09
Log Kow: 2.03 (KowWin estimate)
Melt Pt:
Wat Sol: 224.1 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	68.392
Neutral Organics	: Fish	96-hr	LC50	37.578
Neutral Organics	: Fish	14-day	LC50	68.392
Neutral Organics	: Daphnid	48-hr	LC50	40.349
Neutral Organics	: Green Algae	96-hr	EC50	25.269
Neutral Organics	: Fish	30-day	ChV	4.864
Neutral Organics	: Daphnid	16-day	EC50	2.097
Neutral Organics	: Green Algae	96-hr	ChV	2.571
Neutral Organics	: Fish (SW)	96-hr	LC50	8.734
Neutral Organics	: Mysid Shrimp	96-hr	LC50	10.608
				mg/kg (ppm) dry wt soil
Neutral Organics	: Earthworm	14-day	LC50	325.759 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.

Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

HENRY (v3.10) Program Results:
==========

Bond Est : 7.79E-002 atm-m3/mole
Group Est: 7.05E-002 atm-m3/mole

SMILES : C(C=C)=C
CHEM : 1,3-Butadiene
MOL FOR: C4 H6
MOL WT : 54.09
---------- HENRYWIN v3.10 Results ----------

Experimental Database Structure Match:
Name : 1,3-BUTADIENE
CAS Num : 000106-99-0
Exp HLC : 7.36E-02 atm-m3/mole
Temper : 25 deg C
Exp VP : 2.11E+03 mm Hg
Exp WSol : 7.35E+02 mg/L

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

	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

Henrys LC [VP/WSol estimate using EPI values]:
HLC: 6.827E-002 atm-m3/mole
VP: 2.05E+003 mm Hg
WS: 792 mg/L

BIOWIN (v4.02) Program Results:
==========
SMILES : C(C=C)=C
CHEM : 1,3-Butadiene
MOL FOR: C4 H6
MOL WT : 54.09
---------- BIOWIN v4.02 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) : Biodegrades Fast
Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast

Ready Biodegradability Prediction: YES

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]	0.0062	0.0371
MolWt	*	Molecular Weight Parameter		-0.1609
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.5884

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	-C=CH [alkenyl hydrogen]	0.0285	0.1711
MolWt	*	Molecular Weight Parameter		-1.5616
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.7568

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

AOP Program (v1.91) Results:
==========
SMILES : C(C=C)=C
CHEM : 1,3-Butadiene

MOL FOR: C4 H6
MOL WT : 54.09
------------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS -------------------
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 ----------------------
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 : 66.6 E-12 cm3/molecule-sec
Exper OH Reference: ATKINSON,R (1989)
Exper Ozone rate constant: 8.1 E-18 cm3/molecule-sec
Exper NO3 rate constant : 1.0 E-13 cm3/molecule-sec

PCKOC Program (v1.66) Results:
==========

Koc (estimated): 43.8

SMILES : C(C=C)=C
CHEM : 1,3-Butadiene
MOL FOR: C4 H6
MOL WT : 54.09
---------- PCKOCWIN v1.66 Results ----------

First Order Molecular Connectivity Index	:	1.914
Non-Corrected Log Koc	:	1.6414
Fragment Correction(s) --> NONE	:	---
Corrected Log Koc	:	1.6414

Estimated Koc: 43.79

HYDROWIN Program (v1.67) Results:
==========
SMILES : C(C=C)=C
CHEM : 1,3-Butadiene
MOL FOR: C4 H6
MOL WT : 54.09
---------- HYDROWIN v1.67 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) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)

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

BCF Program (v2.15) Results:
==========
SMILES : C(C=C)=C
CHEM : 1,3-Butadiene

MOL FOR: C4 H6
MOL WT : 54.09

---------- Bcfwin v2.15 ----------

Log Kow (estimated) : 2.03
Log Kow (experimental): 1.99
Log Kow used by BCF estimates: 1.99

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction

Correction(s): Value
No Applicable Correction Factors

Estimated Log BCF = 0.832 (BCF = 6.797)

Volatilization From Water

Chemical Name: 1,3-Butadiene

Molecular Weight : 54.09 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 0.0736 atm-m3/mole (Henry experimental database)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (min) :	45.38	4195
HALF-LIFE (hours) :	0.7563	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

Molecular weight (g/mol)	54.09
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	0.0736
Air-water partition coefficient	3.01002
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	5.74E-003	1.1E-004	0.06
Primary volatilization	1.31E-001	2.4E-003	1.31
Settling volatilization	1.25E-002	2.3E-004	0.12
Aeration off gas	9.46E+000	1.7E-001	94.63
Primary biodegradation	1.80E-003	3.3E-005	0.02

Settling biodegradation	1.89E-005	3.5E-007	0.00
Aeration biodegradation	2.53E-004	4.7E-006	0.00
Final water effluent	3.38E-001	6.3E-003	3.38
Total removal	9.66E+000	1.8E-001	96.62
Total biodegradation	2.07E-003	3.8E-005	0.02

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

(using Biowin/EPA draft method)

PROPERTIES OF: 1,3-Butadiene

Molecular weight (g/mol)	54.09
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	0.0736
Air-water partition coefficient	3.01002
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	1.77	0.39	10.00
-Aeration tank	17.72	0.04	1.00
-Settling tank	17.72	0.04	1.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	1.8E-001	100.00
Primary sludge	4.03E-002	7.5E-004	0.40
Waste sludge	3.00E-003	5.5E-005	0.03
Primary volatilization	1.11E-001	2.0E-003	1.11
Settling volatilization	6.51E-003	1.2E-004	0.07
Aeration off gas	6.35E+000	1.2E-001	63.45
Primary biodegradation	1.52E+000	2.8E-002	15.22
Settling biodegradation	9.84E-002	1.8E-003	0.98
Aeration biodegradation	1.70E+000	3.1E-002	16.97
Final water effluent	1.77E-001	3.3E-003	1.77
Total removal	9.82E+000	1.8E-001	98.23
Total biodegradation	3.32E+000	6.1E-002	33.18

Level III Fugacity Model (Full-Output):

Chem Name : 1,3-Butadiene
Molecular Wt: 54.09
Henry's LC : 0.0736 atm-m3/mole (Henry database)
Vapor Press : 2.05e+003 mm Hg (Mpbpwin program)
Log Kow : 1.99 (Kowwin program)
Soil Koc : 40.1 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	5.74	3.46	1000
Water	90.9	360	1000
Soil	3.04	720	1000
Sediment	0.317	3.24e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	5.27e-011	2.34e+003	117	77.9	3.89
Water	1.26e-006	356	185	11.9	6.16

Soil	2.5e-007	5.94	0	0.198	0
Sediment	1.12e-006	0.138	0.0129	0.0046	0.00043

Persistence Time: 67.7 hr
Reaction Time: 75.3 hr
Advection Time: 674 hr
Percent Reacted: 90
Percent Advected: 10

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 3.462
Water: 360
Soil: 720
Sediment: 3240
Biowin estimate: 3.080 (weeks)

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