



SMILES : O=C
CHEM : Formaldehyde
CAS NUM: 000050-00-0
MOL FOR: C1 H2 O1
MOL WT : 30.03

----- EPI SUMMARY (v3.20) -----

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:

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Log Kow(version 1.67 estimate): 0.35

Experimental Database Structure Match:

Name : Formaldehyde
CAS Num : 000050-00-0
Exp Log P: 0.35
Exp Ref : Hansch,C et al. (1995)

SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Formaldehyde experimental value - constant	0.1210	0.1210
Const		Equation Constant		0.2290

Log Kow = 0.3500

MPBPWIN (v1.42) Program Results:

Experimental Database Structure Match:

Name : FORMALDEHYDE
CAS Num : 000050-00-0
Exp MP (deg C): -92
Exp BP (deg C): -19.1
Exp VP (mm Hg): 3.89E+03 (extrapolated) = 518624.09 Pa
Exp VP (deg C): 25
Exp VP ref : BOUBLIK,T ET AL. (1984)

SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

----- SUMMARY MPBPWIN v1.42 -----

Boiling Point: 9.50 deg C (Adapted Stein and Brown Method)

Melting Point: -113.76 deg C (Adapted Joback Method)
 Melting Point: -108.11 deg C (Gold and Ogle Method)
 Mean Melt Pt : -110.94 deg C (Joback; Gold,Ogle Methods)
 Selected MP: -110.94 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
 (Using BP: -19.10 deg C (exp database))
 (MP not used for liquids)
 VP: 3.67E+003 mm Hg (Antoine Method)
 VP: 3.31E+003 mm Hg (Modified Grain Method)
 VP: 3E+003 mm Hg (Mackay Method)
 Selected VP: 3.49E+003 mm Hg (Mean of Antoine & Grain methods)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CHO (aldehyde)	83.38	83.38
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		281.56
RESULT- corr		BOILING POINT in deg Kelvin		282.66
		BOILING POINT in deg C		9.50

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CHO (aldehyde)	36.90	36.90
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		159.40
		MELTING POINT in deg C		-113.76

Water Sol from Kow (WSKOW v1.41) Results:
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Water Sol: 5.702e+004 mg/L

Experimental Water Solubility Database Match:

Name : FORMALDEHYDE
 CAS Num : 000050-00-0
 Exp WSol : 4E+005 mg/L (20 deg C)
 Exp Ref : PICKRELL,JA ET AL. (1983)

SMILES : O=C
 CHEM : Formaldehyde
 MOL FOR: C1 H2 O1
 MOL WT : 30.03

----- WSKOW v1.41 Results -----

Log Kow (estimated) : 0.35
 Log Kow (experimental): 0.35
 Cas No: 000050-00-0
 Name : Formaldehyde
 Refer : Hansch,C et al. (1995)
 Log Kow used by Water solubility estimates: 0.35

Equation Used to Make Water Sol estimate:

$$\text{Log S (mol/L)} = 0.796 - 0.854 \log \text{Kow} - 0.00728 \text{ MW} + \text{Correction}$$

(used when Melting Point NOT available)

Correction(s): Value

No Applicable Correction Factors

Log Water Solubility (in moles/L) : 0.279
 Water Solubility at 25 deg C (mg/L): 5.702e+004

WATERNT Program (v1.01) Results:
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Water Sol (v1.01 est): 3.9694e+005 mg/L

Experimental Water Solubility Database Match:

Name : FORMALDEHYDE
CAS Num : 000050-00-0
Exp WSol : 4E+005 mg/L (20 deg C)
Exp Ref : PICKRELL,JA ET AL. (1983)

SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Formaldehyde experimental value - constant	0.8720	0.8720
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = 1.1212
Water Solubility (mg/L) at 25 dec C =3.9694e+005

ECOSAR Program (v0.99h) Results:

SMILES : O=C
CHEM : Formaldehyde
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C1 H2 O1
MOL WT : 30.03
Log Kow: 0.35 (KowWin estimate)
Melt Pt:
Wat Sol: 6434 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

Aldehydes

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	1103.201
Aldehydes	: Fish	96-hr	LC50	8.297
Aldehydes	: Daphnid	48-hr	LC50	16.071
Aldehydes	: Green Algae	96-hr	EC50	430.284
Aldehydes	: Fish	32-day	ChV	2.688
Aldehydes	: Green Algae		ChV	16.581

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 6.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 7.0
MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 9.29E-005 atm-m3/mole
Group Est: 6.14E-005 atm-m3/mole

SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

Experimental Database Structure Match:

Name : FORMALDEHYDE
 CAS Num : 000050-00-0
 Exp HLC : 3.37E-07 atm-m3/mole
 Temper : 25 deg C
 Exp Ref : BETTERTON,EA & HOFFMAN,MR (1988)

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	2 Hydrogen to Carbonyl (C=O) Bonds		2.4206
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	2.421

HENRYs LAW CONSTANT at 25 deg C = 9.29E-005 atm-m3/mole = 9.4130925 Pa*m³/mole
 = 3.80E-003 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	1 H2CO	EXPERIMENTAL	2.60
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	2.60

HENRYs LAW CONSTANT at 25 deg C = 6.14E-005 atm-m3/mole
 = 2.51E-003 unitless

Henrys LC [VP/WSol estimate using EPI values]:

HLC: 5.267E-004 atm-m3/mole
 VP: 3.49E+003 mm Hg
 WS: 5.7E+004 mg/L

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

Log Koa: 5.211

SMILES : O=C
 CHEM : Formaldehyde
 MOL FOR: C1 H2 O1
 MOL WT : 30.03

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

Log Koa (octanol/air) estimate: 5.211
 Koa (octanol/air) estimate: 1.625e+005
 Using:
 Log Kow: 0.35 (exp database)
 HenryLC: 3.37e-007 atm-m3/mole (exp database)
 Log Kaw: -4.861 (air/water part.coef.)

 LogKow : 0.35 (exp database)
 LogKow : 0.35 (KowWin estimate)
 Henry LC: 3.37e-007 atm-m3/mole (exp database)
 Henry LC: 9.29e-005 atm-m3/mole (HenryWin bond estimate)

 Log Koa (octanol/air) estimate: 2.770 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:

SMILES : O=C
 CHEM : Formaldehyde
 MOL FOR: C1 H2 O1
 MOL WT : 30.03

----- 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) : Biodegrades Fast
 Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast
 Biowin7 (Anaerobic Model Prediction): Biodegrades Fast
 Ready Biodegradability Prediction: YES

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	0.2846	0.2846
MolWt	*	Molecular Weight Parameter		-0.0143
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		1.0179

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	7.1804	7.1804
MolWt	*	Molecular Weight Parameter		-0.4264
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.9999

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	1	Aldehyde [-CHO]	0.0223	0.0223
MolWt	*	Molecular Weight Parameter		-0.0664
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		3.1551

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	0.1966	0.1966
MolWt	*	Molecular Weight Parameter		-0.0433
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		4.0011

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	1	Aldehyde [-CHO]	0.4114	0.4114
MolWt	*	Molecular Weight Parameter		-0.0893
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		1.0342

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aldehyde [-CHO]	2.7436	2.7436
MolWt	*	Molecular Weight Parameter		-0.8668
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.9879

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	1	Aldehyde [-CHO]	0.1226	0.1226
Const	*	Equation Constant		0.8361
RESULT				0.9587

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

BioHCwin (v1.01) Program Results:

SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

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

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

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 5.19E+005 Pa (3.89E+003 mm Hg)

Log Koa (Koawin est): 5.211

Kp (particle/gas partition coef. (m3/ug)):

Mackay model : 5.78E-012

Octanol/air (Koa) model: 3.99E-008

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 2.09E-010

Mackay model : 4.63E-010

Octanol/air (Koa) model: 3.19E-006

AOP Program (v1.92) Results:

SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

----- SUMMARY (AOP v1.92): HYDROXYL RADICALS -----

Hydrogen Abstraction = 8.1300 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 = 8.1300 E-12 cm3/molecule-sec

HALF-LIFE = 1.316 Days (12-hr day; 1.5E6 OH/cm3)

HALF-LIFE = 15.787 Hrs

----- SUMMARY (AOP v1.91): OZONE REACTION -----

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

Experimental Database Structure Match:

Chem Name : Formaldehyde

CAS Number: 000050-00-0

Exper OH rate constant : 9.37 E-12 cm3/molecule-sec

Exper OH Reference: KWOK,ESC & ATKINSON,R (1994)

Exper Ozone rate constant: 2.1 E-24 cm3/molecule-sec

Exper NO3 rate constant : 5.8 E-16 cm3/molecule-sec

Fraction sorbed to airborne particulates (phi): 3.36E-010 (Junge,Mackay)

Note: the sorbed fraction may be resistant to atmospheric oxidation

PCKOC Program (v1.66) Results:

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Koc (estimated): 1

SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

----- PCKOCWIN v1.66 Results -----

First Order Molecular Connectivity Index : 1.000
Non-Corrected Log Koc : 1.1553
Fragment Correction(s):
 1 Misc (C=O) Group (aliphatic attach).... : -1.2000
Corrected Log Koc : -0.0447
Over Correction Adjustment to Lower Limit Log Koc ... : 0.0000

Estimated Koc: 1

HYDROWIN Program (v1.67) Results:
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SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

----- 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 (v2.17) Results:
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SMILES : O=C
CHEM : Formaldehyde
MOL FOR: C1 H2 O1
MOL WT : 30.03

----- Bcfwin v2.17 -----

Log Kow (estimated) : 0.35
Log Kow (experimental): 0.35
Log Kow used by BCF estimates: 0.35

Equation Used to Make BCF estimate:
Log BCF = 0.50

Correction(s): Value
Correction Factors Not Used for Log Kow < 1

Estimated Log BCF = 0.500 (BCF = 3.162)

Volatilization From Water
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Chemical Name: Formaldehyde

Molecular Weight : 30.03 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 3.37E-007 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 (hours) :	952.6	1.044E+004
HALF-LIFE (days) :	39.69	434.9
HALF-LIFE (years) :	0.1087	1.191

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

(using 10000 hr Bio P,A,S)

PROPERTIES OF: Formaldehyde

Molecular weight (g/mol)	30.03		
Aqueous solubility (mg/l)	0		
Vapour pressure (Pa)	0		
(atm)	0		
(mm Hg)	0		
Henry 's law constant (Atm-m3/mol)	3.37E-007		
Air-water partition coefficient	1.37823E-005		
Octanol-water partition coefficient (Kow)	2.23872		
Log Kow	0.35		
Biomass to water partition coefficient	1.24774		
Temperature [deg C]	25		
Biodeg rate constants (h ⁻¹), half life in biomass (h) and in 2000 mg/L MLSS (h):			
-Primary tank	0.03	24.89	10000.00
-Aeration tank	0.03	24.89	10000.00
-Settling tank	0.03	24.89	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	3.3E-001	100.00
Primary sludge	2.55E-002	8.5E-004	0.25
Waste sludge	1.51E-001	5.0E-003	1.51
Primary volatilization	1.83E-004	6.1E-006	0.00
Settling volatilization	5.00E-004	1.7E-005	0.00
Aeration off gas	1.23E-003	4.1E-005	0.01
Primary biodegradation	1.76E-003	5.9E-005	0.02
Settling biodegradation	5.27E-004	1.8E-005	0.01
Aeration biodegradation	6.94E-003	2.3E-004	0.07
Final water effluent	9.81E+000	3.3E-001	98.13
Total removal	1.87E-001	6.2E-003	1.87
Total biodegradation	9.22E-003	3.1E-004	0.09

Level III Fugacity Model (Full-Output):

Chem Name : Formaldehyde
Molecular Wt: 30.03
Henry's LC : 3.37e-007 atm-m3/mole (Henry database)
Vapor Press : 3.49e+003 mm Hg (Mppwin program)
Log Kow : 0.35 (Kowwin program)
Soil Koc : 0.918 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.13	27.4	1000
Water	44.2	360	1000
Soil	53.5	720	1000
Sediment	0.0826	3.24e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.03e-010	631	250	21	8.32
Water	2.91e-011	997	518	33.2	17.3
Soil	1.21e-009	604	0	20.1	0

Sediment 2.66e-011 0.207 0.0194 0.0069 0.000645

Persistence Time: 390 hr
Reaction Time: 525 hr
Advection Time: 1.53e+003 hr
Percent Reacted: 74.4
Percent Advected: 25.6

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 27.41
Water: 360
Soil: 720
Sediment: 3240
Biowin estimate: 3.155 (weeks)

Advection Times (hr):

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

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