

Carbaryl $C_{12}H_{11}NO_2$ structure



**ASSIGN
BUSTER**

Contents

- Retention Index (Normal Alkane):

Molecular Formula	C ₁₂ H ₁₁ NO ₂
Average mass	201. 221 Da
Density	1. 2±0. 1 g/cm ³
Boiling Point	329. 3±15. 0 °C at 760 mmHg
Flash Point	153. 0±20. 4 °C
Molar Refractivity	59. 0±0. 3 cm ³
Polarizability	23. 4±0. 5 10 ⁻²⁴ cm ³
Surface Tension	45. 1±3. 0 dyne/cm
Molar Volume	170. 0±3. 0 cm ³

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite
- Predicted - ChemAxon
- Predicted - Mcule

- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

142 °C Oxford University Chemical Safety Data (No longer updated) More details

145 °C Jean-Claude Bradley Open Melting Point Dataset 21366

142 °C Jean-Claude Bradley Open Melting Point Dataset 12993, 15072, 8787

144 °C Biosynth Q-200795

141-143 °C LabNetwork LN00337540

142-146 °C BIONET-Key Organics GS-3217

- **Experimental Boiling Point:**

315 °C Oxford University Chemical Safety Data (No longer updated) More details

- **Experimental Flash Point:**

202 °C Oxford University Chemical Safety Data (No longer updated) More details

203 °C Biosynth Q-200795

- **Experimental Gravity:**

1.232 g/mL Fluorochem

203 g/mL BiosynthQ-

200795

1. 232

g/IFluorochem239584

- **Experimental Solubility:**

0.

01% NIOSHFC5950000

- Miscellaneous

- **Appearance:**

colourless solid Oxford University Chemical Safety Data (No longer updated) More details

White or gray, odorless solid. [pesticide] NIOSHFC5950000

- **Stability:**

Stable. Combustible; incompatible with strong oxidizing agents. Oxford University Chemical Safety Data (No longer updated) More details

- **Safety:**

GHS07; GHS08; GHS09 BiosynthQ-200795

H302; H351; H400 BiosynthQ-200795

P101; P273; P281; P301+P312BiosynthQ-200795

Safety glasses, gloves, adequate ventilation. Oxford University Chemical

Data (No longer updated)More details

WarningBiosynthQ-200795

- **First-Aid:**

Eye: Irrigate immediately Skin: Soap wash promptly Breathing: Respirator support Swallow: Medical attention immediatelyNIOSHFC5950000

- **Exposure Routes:**

inhalation, skin absorption, ingestion, skin and/or eye contactNIOSHFC5950000

- **Symptoms:**

Miosis, blurred vision, tear; rhinorrhea (discharge of thin mucus), salivation; sweating; abdominal cramps, nausea, vomiting, diarrhea; tremor; cyanosis; convulsions; irritation skin; possible reproductive effectsNIOSHFC5950000

- **Target Organs:**

ChE inhibitorTargetMoIT0790

respiratory system, central nervous system, cardiovascular system, skin,

cholinesterase, reproductive system NIOSHFC5950000

- **Incompatibility:**

Strong oxidizers, strongly alkaline

pesticides NIOSHFC5950000

- **Personal Protection:**

Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet or contaminated Change:

Daily NIOSHFC5950000

- **Exposure Limits:**

NIOSH REL : TWA 5 mg/m³ OSHA PEL : TWA 5 mg/m³

3 NIOSHFC5950000

- **Bio Activity:**

ChE Target Mol T0790

Neuroscience Target Mol T

0790

- Gas Chromatography

- **Retention Index (Kovats):**

1810 (estimated with error: 89) NIST Spectra mainlib_52624, replib_59654
replib_157293, replib_215734, replib_379930

1871 (Program type: Ramp; Column cl... (show more) ass: Standard non-p

Column diameter: 0.25 mm; Column length: 15 m; Column type: Capillary
rate: 6 K/min; Start T: 100 C; End T: 270 C; CAS no: 63252; Active phase:
Carrier gas: He; Data type: Kovats RI; Authors: Hall, G. L.; Whitehead, W.
Mourer, C. R.; Shibamoto, T., A new gas chromatographic retention index
pesticides and related compounds, J. Hi. Res. Chromatogr. & Chromatogr
Comm., 9, 1986, 266-271.)NIST Spectranist ri

1903 (Program type: Complex; Column... (show more)class: Semi-standa
polar; Column diameter: 0.32 mm; Column length: 30 m; Column type: C
Description: 50C(1min)=> 20C/min=> 150C=> 10C/min=> 280C(4min)
63252; Active phase: HP-5; Phase thickness: 0.25 um; Data type: Kovats
Authors: Tanabe, A.; Mitobe, H.; Kawata, K.; Sakai, M.; Yasuhara, A., New
monitoring system for ninety pesticides and related compounds in river v
solid-phase extraction with determination by gas chromatography/mass
spectrometry, J. AOAC Int., 83(1), 2000, 61-77.)NIST Spectranist ri

1931 (Program type: Isothermal; Col... (show more)umn class: Semi-standa
non-polar; Column diameter: 0.32 mm; Column length: 50 m; Column ty
Capillary; Start T: 200 C; CAS no: 63252; Active phase: Ultra-2; Data type
RI; Authors: Li, L.; Guan, Y.; Zhou, L., Standard Kovats indexes of 20 pest
and their identification in temperature-programmed capillary gas
chromatography., Fenxi Huaxue, 23(1), 1995, 14-19.)NIST Spectranist ri

1910 (Program type: Ramp; Column cl... (show more)ass: Semi-standard
polar; Column diameter: 0.25 mm; Column length: 15 m; Column type: C
Heat rate: 6 K/min; Start T: 100 C; End T: 270 C; CAS no: 63252; Active p
DB-5; Carrier gas: He; Data type: Kovats RI; Authors: Hall, G. L.; Whitehe

E.; Mourer, C. R.; Shibamoto, T., A new gas chromatographic retention index for pesticides and related compounds, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 9, 1986, 266-271.)NIST Spectranist ri

- **Retention Index (Normal Alkane):**

1856 (Program type: Complex; Column... (show more)class: Standard non-polar; Column diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Description: 50C(1min) => 20C/min => 120C => 5C/min => 300C(10min); CAS no: 63252; Active phase: DB-1; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Shimadzu Corporation, Analysis of 124 pesticides with capillary GC-FTD and GC-ECD, 2003.)NIST Spectranist ri

1859.4 (Program type: Complex; Column... (show more)class: Standard non-polar; Column diameter: 0.25 mm; Column length: 50 m; Column type: Capillary; Description: 80C(1min)=> 10C/min => 150C=> 3C/min => 220C => 40C => 280C; CAS no: 63252; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Ma, X.; Li, C.; Liu, W.; Zheng, S., Multi-residue determination of 41 insecticides in garlic by gas chromatography and ion trap mass spectrometry using the selective ion monitoring technique, Rapid Commun. Mass Spectrom., 15, 2001, 15-19.)NIST Spectranist ri

1863.8 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column diameter: 0.2 mm; Column length: 12 m; Column type: Capillary; Description: 18 K/min; Start T: 60 C; End T: 265 C; Start time: 1 min; CAS no: 63252; Active phase: HP-1; Carrier gas: He; Phase thickness: 0.33 um; Data type: Normal alkane RI; Authors: Liao, W.; Joe, T.; Cusick, W. G., Multiresidue screening method for fresh fruits and vegetables with gas chromatographic/mass

spectrometric detection, J. Ass. Offic. Anal. Chem, 74(3), 1991, 554-565.)

Spectranist ri

1903. 5 (Program type: Ramp; Column cl... (show more)ass: Standard no
Column diameter: 0. 2 mm; Column length: 12 m; Column type: Capillary
rate: 18 K/min; Start T: 60 C; End T: 265 C; Start time: 1 min; CAS no: 63
Active phase: HP-1; Carrier gas: He; Phase thickness: 0. 33 um; Data typ
Normal alkane RI; Authors: Liao, W.; Joe, T.; Cusick, W. G., Multiresidue s
method for fresh fruits and vegetables with gas chromatographic/mass
spectrometric detection, J. Ass. Offic. Anal. Chem, 74(3), 1991, 554-565.)

Spectranist ri

1859. 3 (Program type: Complex; Column... (show more)class: Standard
polar; Column diameter: 0. 2 mm; Column length: 25 m; Column type: Ca
Description: 80 0C (0. 5 min) ^ 25 0C/min -> 185 0C ^ 5 0C/min -> 225
min); CAS no: 63252; Active phase: Methyl Silicone; Carrier gas: He; Pha
thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Szeto, S. Y.; F
M., Persistence of pesticide residues in mineral and organic soils in the F
Valley of British Columbia, J. Agric. Food Chem., 39(9), 1991, 1679-1684.

Spectranist ri

1860. 5 (Program type: Ramp; Column cl... (show more)ass: Standard no
Column length: 1. 1 m; Column type: Packed; Heat rate: 8. 5 K/min; Start
End T: 300 C; CAS no: 63252; Active phase: OV-101; Carrier gas: N2; Sub
Chromosorb W HP; Data type: Normal alkane RI; Authors: Saxton, W. L.,
Emergence temperature indices and relative retention times of pesticide
industrial chemicals determined by linear programmed temperature gas

chromatography, J. Chromatogr., 393, 1987, 175-194.)NIST Spectranist ri

1848. 4 (Program type: Complex; Column... (show more)class: Standard non-polar; Column diameter: 0. 247 mm; Column length: 15 m; Column type: Capillary; Description: 1 min at 90 C; 90-150 C at 20 deg/min; 150-250 C at 20 deg/min; hold at 250 C for elution of last component; CAS no: 63252; Active phase: SE-30; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Ripley, B. D.; Braun, H. E., Retention time data for organochlorine, organophosphorus, and organonitrogen pesticides on SE-30 capillary column and application of capillary gas chromatography to pesticide residue analysis, J. Ass. Offic. Anal. Chem, 66(5), 1983, 1084-1095.)NIST Spectranist ri

1865 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column length: 2 m; Column type: Packed; Heat rate: 2. 5 K/min; Start Temperature: 100 C; End T: 200 C; CAS no: 63252; Active phase: SE-30; Substrate: Gas Chromatography; Data type: Normal alkane RI; Authors: Marozzi, E.; Gambaro, V.; Saligari, E.; Marzulli, R.; Lodi, F., Use of the retention index in gas chromatographic studies of pesticides, Anal. Toxicol., 6, 1982, 185-192.)NIST Spectranist ri

1915 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column length: 2 m; Column type: Packed; Heat rate: 2. 5 K/min; Start Temperature: 100 C; End T: 200 C; CAS no: 63252; Active phase: OV-1; Substrate: Gas Chromatography; Data type: Normal alkane RI; Authors: Marozzi, E.; Gambaro, V.; Saligari, E.; Marzulli, R.; Lodi, F., Use of the retention index in gas chromatographic studies of pesticides, Anal. Toxicol., 6, 1982, 185-192.)NIST Spectranist ri

1867. 8 (Program type: Isothermal; Col... (show more)umn class: Standard polar; Column length: 6 ft; Column type: Packed; CAS no: 63252; Active phase: DC-200; Carrier gas: He; Substrate: Chromosorb W HP (80-100 mesh); Data type: Normal alkane RI; Authors: Laski, R. R.; Watts, R. R., Gas chromatography of organonitrogen pesticides, using a nitrogen-specific detection system, J. Offic. Anal. Chem, 55(2), 1973, 328-332.)NIST Spectranist ri

1912 (Program type: Complex; Column... (show more)class: Semi-standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 50 0C(1 min) ^ 25 0C/min -> 125 0C ^ 10 0C/min -> 300 0C (1 min); CAS no: 63252; Active phase: 5 % Phenyl methyl siloxane; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Department of Food Safety, Ministry of Health; Welfare, Analytical methods for residual compositional substances of agricultural chemicals, feed additives and veterinary drugs in foods, 2006.)NIST Spectranist ri

1874 (Program type: Complex; Column... (show more)class: Semi-standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 80C(1min) => 10C/min => 160C (5min) => 3C/min => 240C (25C/min => 280C(10min)); CAS no: 63252; Active phase: DB-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Chen, Hu, X.-Z.; Yao, H.-Y., Determination of 266 pesticide residues in apple juice by matrix solid-phase dispersion and gas chromatography-mass selective detection, J. Chromatogr. A, 1063, 2005, 201-210.)NIST Spectranist ri

1903 (Program type: Complex; Column... (show more)class: Semi-standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary;

Description: 50 0C (1 min) ^ 20 0C/min -> 150 0C ^ 10 0C/min -> 280 0C (10 min); CAS no: 63252; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Kawara, K.; Asada, T.; Oikawa, K.; Tanabe, A., Multiresidue determination of pesticides in sediments by ultrasonically assisted extraction and gas chromatography/mass spectrometry, J. AOAC International, 88(5), 2003, 1440-1451.)NIST Spectranist ri

1923. 3 (Program type: Complex; Column... (show more)class: Semi-stationary, non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 70C(2min) => 25C/min => 150C=> 3C/min => 280C(10min); CAS no: 63252; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Wong, S. E., Webster, M. G.; Bezabeh, D. Z.; Hengel, M. J.; Ngim, K. K.; Krynitsky, A. J., Multiresidue determination of pesticides in malt beverages by capillary gas chromatography with mass spectrometry and selected ion monitoring, J. Food Chem., 52, 2004, 6361-6372.)NIST Spectranist ri

1879. 5 (Program type: Complex; Column... (show more)class: Semi-stationary, non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 50C(1min) => 20C/min => 120C => 5C/min => 300C(10min); CAS no: 63252; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Shimadzu Corporation, Analysis of 124 pesticides with capillary GC-FTD and GC-ECD, J. Chromatogr. A, 1003, 2003.)NIST Spectranist ri

1887. 6 (Program type: Complex; Column... (show more)class: Semi-stationary, non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type:

Capillary; Description: 50 0C (3 min) ^ 25 0C/min -> 125 0C ^ 10 0C/min
0C (25 min); CAS no: 63252; Active phase: HP-5; Carrier gas: He; Phase
thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Lehotay, S. J.
Analysis of pesticide residues in mixed fruit and vegetable extracts by di
sample introduction/gas chromatography/tandem mass spectrometry, J.
Int., 83(3), 2000, 680-697.)NIST Spectranist ri

1899. 3 (Program type: Complex; Column... (show more)class: Semi-stan
non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty
Capillary; Description: 70C(0. 5min) => 10C/min=> 270C(0. 1min) => 2
=> 290C(2min); CAS no: 63252; Active phase: DB-5; Carrier gas: He; Pha
thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Soleas, G. J.;
Hom, K.; Goldberg, D. M., Multiresidue analysis of seventeen pesticides in
by gas chromatography with mass-selective detection, J. Chromatogr. A,
2000, 205-212.)NIST Spectranist ri

1893. 1 (Program type: Complex; Column... (show more)class: Semi-stan
non-polar; Column diameter: 0. 2 mm; Column length: 25 m; Column typ
Capillary; Description: 100C(1min) => 30C/min=> 150C(2min) => 3C/m
205C => 10C/min => 260C(29min); CAS no: 63252; Active phase: SE-54
thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Stan, H.-J., Pe
residue analysis in foodstuffs applying capillary gas chromatography with
spectrometric detection State-of-the-art use of modified DFG-multimetho
and automated data evaluation, J. Chromatogr. A, 892, 2000, 347-377.)N
Spectranist ri

1888. 4 (Program type: Complex; Column... (show more)class: Semi-stan

non-polar; Column diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Description: 50 C (1.13 min) ^ 30 C/min -> 150 C ^ 3 C/min -> 10 C/min -> 250 C (20 min); CAS no: 63252; Active phase: HP-5; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Cook, J.; Engel, Wylie, P.; Quimby, B., Multiresidue screening of pesticides in foods using retention time locking, GC-AED, database search, and GC/MS identification. AOAC Int., 82(2), 1999, 313-326.)NIST Spectranist ri

1914. 7 (Program type: Ramp; Column class: Semi-standard; Column type: non-polar; Column diameter: 0.25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 60 C; End T: 260 C; End time: 12 min; CAS no: 63252; Active phase: DB-5; Carrier gas: He; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Mogadati, P.; Louis, J. B.; Rosen, J. D., Multiresidue determination of pesticides in high-organic-content soils by solid-phase extraction and gas chromatography/mass spectrometry, J. AOAC Int., 82(2), 1999, 705-715.)NIST Spectranist ri

1911. 8 (Program type: Complex; Column class: Semi-standard; Column type: non-polar; Column diameter: 0.32 mm; Column length: 25 m; Column type: Capillary; Description: 50 C(2min) => 20C/min => 150C => 6C/min => 30min); CAS no: 63252; Active phase: NB-54; Phase thickness: 0.25 um; Data type: Normal alkane RI; Authors: Tamura, Y.; Nagayama, T.; Kobayashi, M.; Hiashimoto, T.; Haneishi, N.; Ito, M.; Tomomatsu, T., Simultaneous determination of organonitrogen and carbamate pesticides in foods by an internal standard method based on retention indices in dual-column gas chromatography,

Shokuhin Eiseigaku Zasshi, 39(3), 1998, 225-232.)NIST Spectranist ri

1875. 7 (Program type: Complex; Column... (show more)class: Semi-stan
non-polar; Column diameter: 0. 2 mm; Column length: 25 m; Column typ
Capillary; Description: 85 0C (1 min) ^ 40 0C/min -> 150 0C (2 min) ^ 10
-> 280 0C (20 min); CAS no: 63252; Active phase: HP-5; Carrier gas: He;
thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Holland, P. T.
McNaughton, D. E.; Malcolm, C. P., Multiresidue analysis of pesticides in v
solid-phase extraction, J. AOAC Int., 77(1), 1994, 79-86.)NIST Spectranist

2826 (Program type: Ramp; Column cl... (show more)ass: Standard polar
type: Capillary; CAS no: 63252; Active phase: Carbowax 20M; Data type:
alkane RI; Authors: Tameo, O.; Kiyos, I., Simultaneous determination of p
by capillary gas chromatography, Cannot be traslated (in Japan), 14(2), 1
109-122.)NIST Spectranist ri

Predicted data is generated using the ACD/Labs Percepta Platform -
PhysChem Module

Density:	1. 2±0. 1 g/cm ³
Boiling Point:	329. 3±15. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 7 mmHg at 25°C
Enthalpy of Vaporization:	57. 2±3. 0 kJ/mol
Flash Point:	153. 0±20. 4 °C

Index of Refraction:	1. 611
Molar Refractivity:	59. 0±0. 3 cm ³
#H bond acceptors:	3
#H bond donors:	1
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0
ACD/LogP:	2. 40
ACD/LogD (pH 5. 5):	2. 44
ACD/BCF (pH 5. 5):	41. 95
ACD/KOC (pH 5. 5):	504. 86
ACD/LogD (pH 7. 4):	2. 44
ACD/BCF (pH 7. 4):	41. 95
ACD/KOC (pH 7. 4):	504. 85
Polar Surface Area:	38 Å ²
Polarizability:	23. 4±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	45. 1±3. 0 dyne/cm

Molar Volume: 170. 0±3. 0 cm³

Predicted data is generated using the US Environmental Protection Agency's
EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 2. 35
Log Kow (Exper. database match) = 2. 36
Exper. Ref: Hansch, C et al. (1995)
Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42):
Boiling Pt (deg C): 327. 50 (Adapted Stein & Brown method)
Melting Pt (deg C): 91. 20 (Mean or Weighted MP)
VP (mm Hg, 25 deg C): 5. 33E-005 (Modified Grain method)
MP (exp database): 145 deg C
BP (exp database): 315 deg C
VP (exp database): 1. 36E-06 mm Hg at 25 deg C
Subcooled liquid VP: 2. 09E-005 mm Hg (25 deg C, exp database VP)
Water Solubility Estimate from Log Kow (WSKOW v1. 41):
Water Solubility at 25 deg C (mg/L): 416. 2
log Kow used: 2. 36 (expkow database)
no-melting pt equation used
Water Sol (Exper. database match) = 110 mg/L (22 deg C)
Exper. Ref: PESTICIDE PROP DATABASE
Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 206. 8 mg/L
Wat Sol (Exper. database match) = 110. 00
Exper. Ref: PESTICIDE PROP DATABASE
ECOSAR Class Program (ECOSAR v0. 99h):
Class(es) found: Esters
Henry's Law Constant (25 deg C) [HENRYWIN v3. 10]:
Bond Method : 3. 14E-009 atm-m³/mole
Group Method: Incomplete
Exper Database: 4. 36E-09 atm-m³/mole
Henry's LC [VP/WSol estimate using EPI values]:
3. 391E-008 atm-m³/mole
Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]:
Log Kow used: 2. 36 (exp database)
Log Kaw used: -6. 749 (exp database)
Log Koa (KOAWIN v1. 10 estimate): 9. 109
Log Koa (experimental database): None
Probability of Rapid Biodegradation (BIOWIN v4. 10):
Biowin1 (Linear Model) : 0. 7313
Biowin2 (Non-Linear Model) : 0. 7615
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2. 7078 (weeks-months)
Biowin4 (Primary Survey Model) : 3. 7510 (days)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0. 1280
Biowin6 (MITI Non-Linear Model): 0. 1188
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0. 0885
Ready Biodegradability Prediction: NO
Hydrocarbon Biodegradation (BioHCwin v1. 01):
Structure incompatible with current estimation method!
Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]:
Vapor pressure (liquid/subcooled): 0. 00279 Pa (2. 09E-005 mm Hg)
Log Koa (Koawin est) : 9. 109
Kp (particle/gas partition coef. (m³/ug)): Mackay model : 0. 00108
Octanol/air (Koa) model: 0. 000316
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0. 0374
Mackay model : 0. 0793
Octanol/air (Koa) model: 0. 0246
Atmospheric Oxidation (25 deg C) [AopWin v1. 92]:
Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 25. 9969 E-12
cm³/molecule-sec
Half-Life = 0. 411 Days (12-hr day; 1. 5E6 OH/cm³)
Half-Life = 4. 937 Hrs
Ozone Reaction: No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi): 0. 0584 (Junge, Mackay)
Note: the sorbed fraction may be resistant to atmospheric oxidation
Soil Adsorption Coefficient (PCKOCWIN v1. 66):
Koc : 241. 7
Log Koc: 2. 383
Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]:
Total Kb for pH > 8 at 25 deg C : 4. 680E+000 L/mol-sec
Kb Half-Life at pH 8: 1. 714 days
Kb Half-Life at pH 7: 17. 143 days
Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17):
Log BCF from regression-based method = 1. 117 (BCF = 13. 1)
log Kow used: 2. 36 (expkow database)
Volatilization from Water: Henry LC: 4. 36E-009 atm-m³/mole (Henry experimental database)
Half-Life from Model River: 1. 905E+005 hours (7937

days)Half-Life from Model Lake : 2. 078E+006 hours (8. 659E+004 days)Removal
In Wastewater Treatment: Total removal: 2. 76 percentTotal biodegradation: 0.
10 percentTotal sludge adsorption: 2. 66 percentTotal to Air: 0. 00
percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount
Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0346 9. 87 1000 Water 18. 1
900 1000 Soil 81. 7 1. 8e+003 1000 Sediment 0. 116 8. 1e+003 0 Persistence
Time: 1. 51e+003 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop