

Diisopropyl ether $C_6H_{14}O$ structure



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Contents

- Retention Index (Linear):

Molecular Formula	$C_6H_{14}O$
Average mass	102.175 Da
Density	$0.8 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$68.3 \pm 0.0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$-12.8 \pm 0.0 \text{ }^\circ\text{C}$
Molar Refractivity	$31.5 \pm 0.3 \text{ cm}^3$
Polarizability	$12.5 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	$20.1 \pm 3.0 \text{ dyne/cm}$
Molar Volume	$134.7 \pm 3.0 \text{ cm}^3$

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

- Experimental Physico-chemical Properties
 - **Experimental Melting Point:**
 - 86 °C Jean-Claude Bradley Open Melting Point Dataset13355
 - 86. 8 °C Jean-Claude Bradley Open Melting Point Dataset20515
 - 0. 725 °C LabNetworkLN00163172
 - **Experimental Boiling Point:**
 - 154 F (67. 7778 °C) NIOSHTZ5425000
 - 68 °C LabNetworkLN00163172
 - **Experimental Ionization Potent:**
 - 9. 2
 - Ev NIOSHTZ5425000
 - **Experimental Vapor Pressure:**
 - 119
 - mmHg NIOSHTZ5425000
 - **Experimental Flash Point:**
 - 18 F (-27. 7778

°C)NIOSH5425000

-28-18

°CLabNetworkLN00163172

- **Experimental Freezing Point:**

-76 F (-60

°C)NIOSH5425000

- **Experimental Gravity:**

20 g/mL Merck Millipore 1176, 4456

20 g/L Merck Millipore 1176, 4456,

845123, 800866

- **Experimental Refraction Index:**

1. 3684 Alfa

Aesar L13215

- **Experimental Solubility:**

0. 2% NIOSH 5425000

-1. 10 Egon Willighagen [http://dx. doi. org/10.](http://dx.doi.org/10.1021/ci050282s)

1021/ci050282s

- Miscellaneous

- **Appearance:**

Colorless liquid with a sharp, sweet, ether-like odor.

NIOSHTZ5425000

- **Safety:**

DANGER: FLAMMABLE, causes CNS effects, irritates skin & eyesAlfa

AesarL13215

- **First-Aid:**

Eye: Irrigate immediately Skin: Soap wash promptly Breathing: Respirator support Swallow: Medical attention immediatelyNIOSHTZ5425000

- **Exposure Routes:**

inhalation, ingestion, skin and/or eye

contactNIOSHTZ5425000

- **Symptoms:**

Irritation eyes, skin, nose; respiratory discomfort; dermatitis; in animals: drowsiness, dizziness, unconsciousness, narcosisNIOSHTZ5425000

- **Target Organs:**

Eyes, skin, respiratory system, central nervous systemNIOSHTZ5425000

- **Incompatibility:**

Strong oxidizers, acids [Note: Unstable peroxides may form on long cont

air.]NIOSHTZ5425000

- **Personal Protection:**

Skin: Prevent skin contact Eyes: Prevent eye contact Wash skin: When contaminated Remove: When wet (flammable) Change: No recommendationNIOSHTZ5425000

- **Exposure Limits:**

NIOSH REL : TWA 500 ppm (2100 mg/m³) OSHA PEL : TWA 500 ppm (2100 mg/m³)NIOSHTZ5425000

- Gas Chromatography

- **Retention Index (Kovats):**

602 (Program type: Complex; Column... (show more)class: Standard non
Column diameter: 0.2 mm; Column length: 100 m; Column type: Capilla
Description: 5C(10min)=> 5C/min=> 50C(48min)=> 1. 5C/min=> 195C
CAS no: 108203; Active phase: Petrocol DH-100; Carrier gas: He; Data ty
Kovats RI; Authors: Haagen-Smit Laboratory, Procedure for the detailed
hydrocarbon analysis of gasolines by single column high efficiency (capil
column gas chromatography, SOP NO. MLD 118, Revision No. 1. 1, Califo
Environmental Protection Agency, Air Resources Board, El Monte, Californ
1997, 22.)NIST Spectranist ri

593 (Program type: Isothermal; Col... (show more)umn class: Standard n
Column length: 3 m; Column type: Packed; Start T: 120 C; CAS no: 10820
Active phase: SE-30; Carrier gas: N₂; Substrate: Supelcoport; Data type:

RI; Authors: Garcia-Raso, A.; Martinez-Castro, I.; Paez, M. I.; Sanz, J.; Garcia-Raso, J.; Saura-Calixto, F., Gas Chromatographic Behaviour of Carbohydrate Trimethylsilyl Ethers. I. Aldopentoses, J. Chromatogr., 398, 1987, 9-20.)NIST Spectranist ri

590 (Program type: Isothermal; Column class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 108203; Active phase: SE-30; Carrier gas: Ar; Substrate: Gas Chrom Q (80-100 mesh); Data type: Kovats RI; Authors: Tiess, D., Gaschromatographische Retentionsindices von 125 leicht- bis mittelfluchtigen organischen Substanzen: toxikologisch-analytischer Relevanz auf SE-30, Wiss. Z. Wilhelm-Pieck-Universität Rostock Math. Naturwiss. Reihe, 33, 1984, 6-9.)NIST Spectranist ri

594 (Program type: Isothermal; Column class: Standard non-polar; Column length: 2 m; Column type: Packed; Start T: 100 C; CAS no: 108203; Active phase: SE-30; Substrate: Gaschrom Q; Data type: Kovats RI; Author: Winskowski, J., Gaschromatographische Identifizierung von Stoffen anhand der Retentionsindexziffern und unterschiedlichen Detektoren, Chromatographia, 17(3), 1964, 160-165.)NIST Spectranist ri

624 (Program type: Isothermal; Column class: Semi-standard non-polar; Column type: Packed; Start T: 200 C; CAS no: 108203; Active phase: Porapack Q; Carrier gas: N2; Data type: Kovats RI; Authors: Goebel, K.-J., Gaschromatographische Identifizierung Niedrig Siedender Substanzen Mittels der Retentionsindices und Rechnerhilfe, J. Chromatogr., 235, 1982, 119-127.)NIST Spectranist ri

563 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column type: Packed; Start T: 120 C; CAS no: 108203; Active phas
Apiezon L; Substrate: Celite 545; Data type: Kovats RI; Authors: Bogoslov
N.; Anvaer, B. I.; Vigdergauz, M. S., Chromatographic constants in gas
chromatography (in Russian), Standards Publ. House, Moscow, 1978, 192
Spectranist ri

564 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column type: Packed; Start T: 160 C; CAS no: 108203; Active phas
Apiezon L; Substrate: Celite 545; Data type: Kovats RI; Authors: Bogoslov
N.; Anvaer, B. I.; Vigdergauz, M. S., Chromatographic constants in gas
chromatography (in Russian), Standards Publ. House, Moscow, 1978, 192
Spectranist ri

570 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column length: 2. 25 m; Column type: Packed; Start T: 70 C; CAS n
108203; Active phase: Apiezon L; Substrate: Celite; Data type: Kovats RI,
Authors: Wehrli, A.; Kovats, E., Gas-chromatographische Charakterisierung
organischer Verbindungen. Teil 3: Berechnung der Retentionsindices
aliphatischer, alicyclischer und aromatischer Verbindungen, Helv. Chim. A
1959, 2709-2736., Program type: Isothermal; Col... (show more)umn clas
standard non-polar; Column type: Packed; Start T: 70 C; CAS no: 108203
phase: Apiezon L; Data type: Kovats RI; Authors: Bogoslovsky, Yu. N.; An
I.; Vigdergauz, M. S., Chromatographic constants in gas chromatography
Russian), Standards Publ. House, Moscow, 1978, 192.)NIST Spectranist ri

565 (Program type: Isothermal; Col... (show more)umn class: Semi-stand

polar; Column length: 2. 1 m; Column type: Packed; Start T: 130 C; CAS no: 108203; Active phase: Apiezon M; Carrier gas: N2; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Golovnya, R. V.; Garbuzov, V. G., Effect of heteroatom in aliphatic sulfur- and oxygen-containing compounds on the values of the retention indices in gas chromatography, *Izv. Akad. Nauk SSSR Ser. Khim.*, 1974, 1519-1521, In original 1599-1601.)NIST Spectramainlib_229501, replib_19939, replib_19940, nist ri

568 (Program type: Isothermal; Column class: Semi-standard; Column diameter: 0. 25 mm; Column length: 2. 25 m; Column type: Packed; Start T: 130 C; CAS no: 108203; Active phase: Apiezon L; Substrate: Celite; Data type: Kovats RI; Authors: Wehrli, A.; Kovats, E., Gas-chromatographische Charakterisierung organischer Verbindungen. Teil 3: Berechnung der Retentionsindices aliphatischer, alicyclischer und aromatischer Verbindungen, *Helv. Chim. Acta.*, 1959, 2709-2736.)NIST Spectranist ri

652 (Program type: Isothermal; Column class: Standard; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 120 C; CAS no: 108203; Active phase: Carbowax 20M; Carrier gas: N2; Substrate: Supelcoport; Data type: Kovats RI; Authors: Garcia-Raso, A.; M. Castro, I.; Paez, M. I.; Sanz, J.; Garcia-Raso, J.; Saura-Calixto, F., Gas Chromatographic Behaviour of Carbohydrate Trimethylsilyl Ethers. I. Aldopentoses, *J. Chromatogr.*, 398, 1987, 9-20.)NIST Spectranist ri

679 (Program type: Isothermal; Column class: Standard; Column length: 2 m; Column type: Packed; Start T: 75 C; CAS no: 108203; Active phase: Carbowax 20M; Carrier gas: N2; Substrate: Kieselgur (60-100 mesh)

type: Kovats RI; Authors: Goebel, K.-J., Gaschromatographische Identifizierung
Niedrig Siedender Substanzen Mittels Retentionsindices und Rechnerhilfen
Chromatogr., 235, 1982, 119-127.)NIST Spectranist ri

667 (Program type: Isothermal; Col... (show more)umn class: Standard p
Column length: 3 m; Column type: Packed; Start T: 180 C; CAS no: 10820
Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 m
Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Go
L., Gas-liquid chromatography of some aliphatic and heterocyclic mono-
polyfunctional amines. VII. Retention indices of amines in some polar and
unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973
63.)NIST Spectranist ri

670 (Program type: Isothermal; Col... (show more)umn class: Standard p
Column length: 3 m; Column type: Packed; Start T: 150 C; CAS no: 10820
Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 m
Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Go
L., Gas-liquid chromatography of some aliphatic and heterocyclic mono-
polyfunctional amines. VII. Retention indices of amines in some polar and
unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973
63.)NIST Spectranist ri

682 (Program type: Isothermal; Col... (show more)umn class: Standard p
Column length: 3 m; Column type: Packed; Start T: 120 C; CAS no: 10820
Active phase: PEG-2000; Carrier gas: He; Substrate: Celite 545 (44-60 m
Data type: Kovats RI; Authors: Anderson, A.; Jurel, S.; Shymanska, M.; Go
L., Gas-liquid chromatography of some aliphatic and heterocyclic mono-

polyfunctional amines. VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR Zinat. Akad. Vestis Kim. Ser., , 1973

63.)NIST Spectranist ri

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

590 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar
Column type: Capillary; CAS no: 108203; Active phase: SE-30; Data type: Normal
alkane RI; Authors: Vinogradov, B. A., Production, composition, properties and
application of essential oils, 2004.)NIST Spectranist ri

598. 8 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar
Column diameter: 0. 53 mm; Column length: 30 m; Column type: Capillary
rate: 10 K/min; Start T: 40 C; End T: 260 C; Start time: 5 min; CAS no: 108203
Active phase: DB-1; Carrier gas: He; Phase thickness: 3 um; Data type: Normal
alkane RI; Authors: J&W Scientific, Solvent Retention Data, 2003.)NIST
Spectranist ri

568 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar
Column type: Capillary; CAS no: 108203; Active phase: Methyl Silicone; Data
type: Normal alkane RI; Authors: Du, X., Quantitative structure-property
relationship study on analysis of retention index of organic compound in
chromatography, Chemical World (Chinese), 42(8), 2001, 403-406.)NIST
Spectranist ri

599. 8 (Program type: Complex; Column... (show more)class: Standard non-polar
Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary
Description: 35C(4min) => 4C/min => 130C => 25C/min => 200C(5min)

no: 108203; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness:
Data type: Normal alkane RI; Authors: Miermans, C. J. H.; van der Velde,
Frintrop, P. C. M., Analysis of volatile organic compounds, using the purg
trap injector coupled to a gas chromatograph/ion-trap mass spectromete
Review of the results in Dutch surface water of the Rhine, Meuse, Northe
Area and Westerscheldt, over the period 1992-1997, Chemosphere, 40, 2
48.)NIST Spectranist ri

600. 6 (Program type: Ramp; Column cl... (show more)ass: Standard non
Column diameter: 0. 53 mm; Column type: Capillary; Heat rate: 4 K/min;
35 C; End T: 220 C; End time: 2 min; Start time: 10 min; CAS no: 108203
phase: RTX-1; Carrier gas: He; Phase thickness: 3 um; Data type: Normal
RI; Authors: Restek, Restek International, 1999 Product Guide, 1(1), 1999
591, In original 578-591.)NIST Spectranist ri

598 (Program type: Complex; Column... (show more)class: Standard non
Column diameter: 0. 53 mm; Column length: 60 m; Column type: Capilla
Description: 40C(6min)=> 5C/min=> 80C=> 10C/min=> 200C; CAS no:
Active phase: SPB-1; Carrier gas: He; Phase thickness: 5 um; Data type: N
alkane RI; Authors: Flanagan, R. J.; Streete, P. J.; Ramsey, J. D., Volatile S
Abuse, UNODC Technical Series, No 5, United Nations, Office on Drugs and
Crime, Vienna International Centre, PO Box 500, A-1400 Vienna, Austria,
56.)NIST Spectranist ri

596 (Program type: Ramp; Column cl... (show more)ass: Standard non-po
Column type: Capillary; CAS no: 108203; Active phase: Methyl Silicone; D
type: Normal alkane RI; Authors: Zenkevich, I. G.; Korolenko, L. I.; Khrale

N. B., Desorption with solvent vapor as a method of sample preparation in
sorption preconcentration of organic-compounds from the air of a working
and from industrial-waste gases, J. Appl. Chem. USSR (Engl. Transl.), 50(1995,
1995, 937-944.)NIST Spectranist ri

594 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar
Column type: Capillary; CAS no: 108203; Active phase: OV-1; Data type:
alkane RI; Authors: Ramsey, J. D.; Flanagan, R. J., Detection and Identification
Volatile Organic Compounds in Blood by Headspace Gas Chromatography
Aid to the Diagnosis of Solvent Abuse, J. Chromatogr., 240, 1982, 423-44
Spectranist ri

602. 4 (Program type: Ramp; Column cl... (show more)ass: Semi-standard
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
CAS no: 108203; Active phase: RTX-5; Carrier gas: He; Phase thickness: 0
um; Data type: Normal alkane RI; Authors: Wentworth, W. E.; Helias, N.; J
A.; Chen, E. C. M.; Stearns, S. D., Multiple detector responses for gas
chromatography peak identification, J. Chromatogr. A, 795, 1998, 319-34
Spectranist ri

603 (Program type: Complex; Column... (show more)class: Semi-standard
polar; Column diameter: 0. 25 mm; Column length: 40 m; Column type: C
Description: 30 0C (1 min) ^ 15 0C/min -> 45 0C ^ 3 0C/min -> 120 0C;
108203; Active phase: CP Sil 8 CB; Carrier gas: He; Phase thickness: 0. 2
Data type: Normal alkane RI; Authors: Weller, J.-P.; Wolf, M.,
Massenspektroskopie und Headspace-GC, Beitr. Gerichtl. Med., 47, 1989

532.)NIST Spectranist ri

649 (Program type: Ramp; Column cl... (show more)ass: Standard polar;
type: Capillary; CAS no: 108203; Active phase: Carbowax 20M; Data type:
alkane RI; Authors: Vinogradov, B. A., Production, composition, properties
application of essential oils, 2004.)NIST Spectranist ri

662 (Program type: Ramp; Column cl... (show more)ass: Standard polar;
type: Capillary; CAS no: 108203; Active phase: Polyethylene Glycol; Data
Normal alkane RI; Authors: Zenkevich, I. G.; Korolenko, L. I.; Khralenkova
Desorption with solvent vapor as a method of sample preparation in the
preconcentration of organic-compounds from the air of a working area and
industrial-waste gases, J. Appl. Chem. USSR (Engl. Transl.), 50(10), 1995,
944.)NIST Spectranist ri

- **Retention Index (Linear):**

655. 4 (Program type: Ramp; Column cl... (show more)ass: Standard polar;
Column diameter: 0. 27 mm; Column length: 62 m; Column type: Capilla
rate: 2 K/min; Start T: 90 C; CAS no: 108203; Active phase: PEG-20M; Da
Linear RI; Authors: Wang, T.; Sun, Y., Correlation of Retention Indices obt
with Two Temperature Programmes, J. Chromatogr., 330, 1985, 167-171,
original 167-171.)NIST Spectranist ri

657 (Program type: Ramp; Column cl... (show more)ass: Standard polar;
diameter: 0. 27 mm; Column length: 62 m; Column type: Capillary; Heat
K/min; Start T: 80 C; CAS no: 108203; Active phase: PEG-20M; Data type
RI; Authors: Wang, T.; Sun, Y., Correlation of Retention Indices obtained v

Temperature Programmes, J. Chromatogr., 330, 1985, 167-171, In original
171.)NIST Spectranist ri

658. 3 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 27 mm; Column length: 62 m; Column type: Capilla
rate: 4 K/min; Start T: 70 C; CAS no: 108203; Active phase: PEG-20M; Da
Linear RI; Authors: Wang, T.; Sun, Y., Correlation of Retention Indices obt
with Two Temperature Programmes, J. Chromatogr., 330, 1985, 167-171,
original 167-171.)NIST Spectranist ri

659 (Program type: Ramp; Column cl... (show more)ass: Standard polar;
diameter: 0. 27 mm; Column length: 62 m; Column type: Capillary; Heat
K/min; Start T: 70 C; CAS no: 108203; Active phase: PEG-20M; Data type
RI; Authors: Wang, T.; Sun, Y., Correlation of Retention Indices obtained v
Temperature Programmes, J. Chromatogr., 330, 1985, 167-171, In original
171.)NIST Spectranist ri

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

Density:	0. 8±0. 1 g/cm ³
Boiling Point:	68. 3±0. 0 °C at 760 mmHg
Vapour Pressure:	152. 3±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	29. 1±0. 0 kJ/mol
Flash Point:	-12. 8±0. 0 °C

Index of Refraction:	1. 384
Molar Refractivity:	31. 5±0. 3 cm ³
#H bond acceptors:	1
#H bond donors:	0
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0
ACD/LogP:	1. 68
ACD/LogD (pH 5. 5):	1. 88
ACD/BCF (pH 5. 5):	15. 74
ACD/KOC (pH 5. 5):	250. 30
ACD/LogD (pH 7. 4):	1. 88
ACD/BCF (pH 7. 4):	15. 74
ACD/KOC (pH 7. 4):	250. 30
Polar Surface Area:	9 Å ²
Polarizability:	12. 5±0. 5 10 ⁻²⁴ cm ³

Surface Tension: 20. 1±3. 0 dyne/cm

Molar Volume: 134. 7±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) = 1. 88Log Kow (Exper. database match) = 1. 52Exper. Ref: Funasaki, N et al. (1985)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 67. 34 (Adapted Stein & Brown method)Melting Pt (deg C): -98. 95 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 151 (Mean VP of Antoine & Grain methods)MP (exp database): -86. 8 deg CBP (exp database): 68. 5 deg CVP (exp database): 1. 49E+02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 5800log Kow used: 1. 52 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 8800 mg/L (20 deg C)Exper. Ref: HEITMANN, W ET AL (1987)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 15525 mg/LWat Sol (Exper. database match) = 8800. 00Exper. Ref: HEITMANN, W ET AL (1987)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenry's Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 68E-003 atm-m³/moleGroup Method: 4. 99E-003 atm-m³/moleExper Database: 2. 28E-03 atm-m³/moleHenry's LC [VP/WSol estimate using EPI values]: 3. 500E-003 atm-m³/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 52 (exp database)Log Kaw used: -1. 031 (exp database)Log Koa (KOAWIN v1. 10 estimate): 2. 551Log Koa (experimental database): 2. 660Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 3515Biowin2 (Non-Linear Model) : 0. 1334Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9647 (weeks)Biowin4 (Primary Survey Model) : 3. 6906 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3099Biowin6 (MITI Non-Linear Model): 0. 3423Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 0712Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 1. 99E+004 Pa (149 mm Hg)Log Koa (Exp database): 2. 660Kp (particle/gas partition coef. (m³/ug)): Mackay model : 1. 51E-010 Octanol/air (Koa) model: 1. 12E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 5. 45E-009 Mackay model : 1. 21E-008 Octanol/air (Koa) model: 8. 98E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 24. 3371 E-12 cm³/molecule-secHalf-Life = 0. 439 Days (12-hr day; 1. 5E6 OH/cm³)Half-Life = 5. 274 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 8. 77E-009 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 10. 5Log Koc: 1. 021 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Rate constants can NOT be estimated for this structure! Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0. 470 (BCF = 2. 954)log Kow used: 1.

<https://assignbuster.com/diisopropyl-ether-c6h14o-structure/>

52 (expkow database)Volatilization from Water: Henry LC: 0. 00228 atm-m3/mole
(Henry experimental database)Half-Life from Model River: 1. 291 hoursHalf-
Life from Model Lake : 98. 84 hours (4. 118 days)Removal In Wastewater
Treatment: Total removal: 48. 59 percentTotal biodegradation: 0. 06
percentTotal sludge adsorption: 1. 14 percentTotal to Air: 47. 40
percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount
Half-Life Emissions(percent) (hr) (kg/hr)Air 19. 4 25. 2 1000 Water 61 360
1000 Soil 19. 5 720 1000 Sediment 0. 147 3. 24e+003 0 Persistence Time: 108
hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop