2,4-di-t-butylphenol c14h22o structure

Contents

- Retention Index (Linear):

Molecular Formula	$C_{14}H_{22}O$
Average mass	206. 324 Da
Density	0. 9±0. 1 g/cm ^{3}
Boiling Point	265. 5±9. 0 °C at 760 mmHg
Flash Point	115. 0±0. 0 °C
Molar Refractivity	64. 9±0. 3 cm ^{3}
Polarizability	25. 7±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	30. 1±3. 0 dyne/cm
Molar Volume	221. 2±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties
    - **Experimental Melting Point:**

      56 °CTCID0229

      53-57 °CAlfa Aesar

      52-57 °COxford University Chemical Safety Data (No longer updated)More details

      55-59 °CMerck Millipore3381, 820422

      55 °CJean-Claude Bradley Open Melting Point Dataset1554

      54. 5 °CJean-Claude Bradley Open Melting Point Dataset15178

      56. 5 °CJean-Claude Bradley Open Melting

Point Dataset20797

53-57 °CAlfa

AesarA18509

54 °CBiosynthQ-

200191

56-58

°CLabNetworkLN00226

610

- **Experimental Boiling Point:**

  265 °CAlfa Aesar

  265 °COxford

  University Chemical

  Safety Data (No longer

  updated)More details

  265 °CAlfa

  AesarA18509

  265

  °CLabNetworkLN00226

  610

- **Experimental Flash Point:**

  129 °CAlfa Aesar

  115 °COxford

  University Chemical

  Safety Data (No longer

  updated)More details

  129 °CAlfa Aesar

  115 °CBiosynthQ-

  200191

  129 °F (53. 8889

  °C)Alfa AesarA18509

  239

  °CLabNetworkLN00226

  610

- **Experimental Gravity:**

  0. 887 g/mLAlfa

  AesarA18509

  115 g/mLBiosynthQ-

  200191

- Predicted Physico-chemical Properties

- **Predicted Melting Point:**

  54-59 °CJ&K

  Scientific244431

  56 °CTCI

  56 °CTCID0229

- Miscellaneous

  - **Appearance:**

    light yellow

    crystalsOxford

    University Chemical

    Safety Data (No longer

    updated)More details

    Not

    AvailableNovochemy[N

    C-30164]

  - **Stability:**

    Stable. Combustible.

    Incompatible with acid

    chlorides, oxidizing

    agents, acid

    anhydrides, copper,

    copper alloys, bases,

brass. Oxford

University Chemical

Safety Data (No longer

updated)More details

- **Toxicity:**

  IPR-MUS LD50 25mg

  kg-1Oxford University

  Chemical Safety Data

  (No longer

  updated)More details

- **Safety:**

  20/21/22Novochemy[N

  C-30164]

  20/21/36/37/39Novoch

  emy[NC-30164]

  26-37Alfa AesarA18509

  26-37-57-60Alfa

  AesarA18509

  36/37/38-51/53Alfa

  AesarA18509

  9Alfa AesarA18509

GHS07;

GHS09BiosynthQ-

200191

GHS07;

GHS09Novochemy[NC-

30164]

H315; H319; H335;

H410BiosynthQ-

200191

H315-H319-H335-

H411Alfa AesarA18509

H332;

H403Novochemy[NC-

30164]

P261; P273;

P305+P351+P338;

P501BiosynthQ-200191

P261-P280-

P305+P351+P338-

P304+P340-P405-

P501aAlfa

AesarA18509

P301+P310;

P337+P313Novochemy

[NC-30164]

R22Novochemy[NC-

30164]

Safety glasses,

adequate ventilation.

Oxford University

Chemical Safety Data

(No longer

updated)More details

WarningAlfa

AesarA18509

WarningBiosynthQ-

200191

WarningNovochemy[NC

-30164]

WARNING: Irritates

lungs, eyes, skinAlfa

AesarA18509

- Gas Chromatography

  - **Retention Index (Kovats):**

    1555 (estimated with

    error: 70)NIST

    Spectramainlib_228966

    , replib_22572,

    replib_133233

1519 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 3 m; Column type: Packed; Start T: 523 K; CAS no: 96764; Active phase: SE-30; Carrier gas: He; Substrate: N_AW_HMDS; Data type: Kovats RI; Authors: Verevkin, S. P.; Nesterov, O. A.; Rempel, P. D.; Synkova, N. V.; Shashkin, N. P., Chromatographic determination of the products of condensation of alkylphenols with formic aldehyde, Zh. Anal. Khim., 43, 1990, 760-761.)NIST

Spectranist ri

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

  1494 (Program type:

  Ramp; Column cl...

  (show more)ass:

  Standard non-polar;

  Column diameter: 0. 25

  mm; Column length:

  150 m; Column type:

  Capillary; Heat rate: 1

  K/min; Start T: 40 C;

  End T: 300 C; CAS no:

  96764; Active phase:

  Petrocol DH; Phase

  thickness: 1. 0 um;

  Data type: Normal

  alkane RI; Authors:

  Sojak, L.; Kubinec, R.;

  Jurdakova, H.;

  Hajekova, E.; Bajus, M.,

  GC-MS of polyethylene

  and polypropylene

  thermal cracking

  produxts, Petroleum &

  Coal, 48(1), 2006, 1-

14.)NIST Spectranist ri

1502 (Program type: Complex; Column... (show more)class: Standard non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Description: 0C (3min) => 3C/min => 50C => 5C/min => 220C (30min); CAS no: 96764; Active phase: CP-Sil5 CB MS; Phase thickness: 0. 4 um; Data type: Normal alkane RI; Authors: Tirillini, B.; Verdelli, G.; Paolocci, F.; Ciccioli, P.; Frattoni, M., The volatile organic compounds from the mycelium of Tuber borchii Vitt., Phytochemistry, 55,

2000, 983-985.)NIST

Spectranist ri

1519 (Program type:

Complex; Column…

(show more)class:

Semi-standard non-

polar; Column

diameter: 0. 25 mm;

Column length: 30 m;

Column type: Capillary;

Description: 40C

(10min) => 3C/min =>

120C => 10C/min =>

250C (5min); CAS no:

96764; Active phase:

HP-5MS; Carrier gas:

He; Phase thickness: 0.

25 um; Data type:

Normal alkane RI;

Authors: Ansorena, D.;

Gimeno, O.; Astiasaran,

I.; Bello, J., Analysis of

volatile compounds by

GC-MS of a dry

fermented sausage:

chorizo de Pamplona,

Food Res. Int., 34,

2001, 67-75., Program

type: Complex;

Column... (show

more)class: Semi-

standard non-polar;

Column diameter: 0. 25

mm; Column length: 30

m; Column type:

Capillary; Description:

50 0C (5 min) ^ 2

0C/min -> 100 0C (5

min) ^ 5 0C/min ->

300 0C; CAS no:

96764; Active phase:

RTX-5 MS; Carrier gas:

Helium; Phase

thickness: 0. 25 um;

Data type: Normal

alkane RI; Authors:

Mebazaa, R.;

Mahmoudi, A.; Fouchet,

M.; Dos Santos, M.;

Kamissoko, F.; Nafti, A.;

Ben Cheikh, R.; Rega,

B.; Camel, V., Characterization of volatile compounds in Tunisian fenugreek seeds, Food Chem., 115, 2009, 1326-1336., Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; CAS no: 96764; Active phase: HP-5; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Zhao, Y.; Li, J.; Xu, Y.; Duan, H.; Fan, W.; Zhao, G., EXtraction, preparation and identification of volatile compounds in Changyu XO brandy, Chinese J. Chromatogr.,

26(2), 2008, 212-

222.)NIST Spectranist ri

1509 (Program type:

Complex; Column…

(show more)class:

Semi-standard non-

polar; Column

diameter: 0. 25 mm;

Column length: 30 m;

Column type: Capillary;

Description: 40 0C (2

min) ^ 5 0C/min -> 80

0C ^ 7 oC/min -> 160

0C ^ 9 0C/min -> 200

0C ^ 20 0C/min -> 280

0C (10 min); CAS no:

96764; Active phase:

HP-5; Phase thickness:

0. 25 um; Data type:

Normal alkane RI;

Authors: Zhao, Y.; Li, J.;

Xu, Y.; Duan, H.; Fan,

W.; Zhao, G.,

EXtraction, preparation

and identification of

volatile compounds in Changyu XO brandy, Chinese J. Chromatogr., 26(2), 2008, 212-222.)NIST Spectranist ri

2312 (Program type: Complex; Column... (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 50 0C ^ 2 0C/min -> 100 0C (5 min) ^ 5 0C/min -> 250 0C; CAS no: 96764; Active phase: DB-FFAP; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Mebazaa, R.; Mahmoudi, A.; Fouchet, M.; Dos Santos, M.;

Kamissoko, F.; Nafti, A.; Ben Cheikh, R.; Rega, B.; Camel, V., Characterization of volatile compounds in Tunisian fenugreek seeds, Food Chem., 115, 2009, 1326-1336.)NIST Spectranist ri

2330 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40 0C (4 min) ^ 3 0C/min -> 50 0C ^ 5 0C/min -> 120 0C ^ 7 0C/min -> 175 0C ^ 10 0C/min -> 230 0C (8 min); CAS no: 96764; Active phase: DB-Wax; Carrier gas:

Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Yongsheng, T.; Hua, L.; Hua, W.; Li, Z., Volatile composition of young Cabernet Savignon red wine from Changli Counti (China), J. Food Composition and Analysis, 21, 2008, 689-694., Program type: Complex; Column... (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40C(3min) => 4C/min => 160C => 7C/min => 230C (8min); CAS no: 96764; Active phase: DB-Wax; Carrier gas: He; Phase

thickness: 0. 25 um;

Data type: Normal

alkane RI; Authors: Li,

H.; Tao, Y.-S.; Wang,

H.; Zhang, L., Impact

odorants of

Chardonnay dry white

wine from Changli

County (China), Eur.

Food Res. Technol., ,

2007.)NIST Spectranist

ri

2270 (Program type:

Ramp; Column cl…

(show more)ass:

Standard polar; Column

diameter: 0. 25 mm;

Column length: 30 m;

Column type: Capillary;

Heat rate: 10 K/min;

Start T: 40 C; End T:

220 C; End time: 10

min; Start time: 5 min;

CAS no: 96764; Active

phase: RTX-Wax;

Carrier gas: He; Phase thickness: 0. 5 um; Data type: Normal alkane RI; Authors: Prososki, R. A.; Etzel, M. R.; Rankin, S. A., Solvent type affects the number, distribution, and relative quantities of volatile compounds found in sweet whey powder, J. Dairy Sci., 90, 2007, 523-531.)NIST Spectranist ri

2277 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 60 0C (3 min) ^ 2 0C/min -> 220 0C ^ 3 0C/min ->

245 0C (20 min); CAS no: 96764; Active phase: DB-Wax; Carrier gas: Hydrogen; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Selli, S., Volatile constituents of orange obtained from moro oranges (Citrus Sinensis L. Osbeck), J. Food Quality, 30, 2007, 330-341.)NIST Spectranist ri

2315 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Description: 40 0C (5 min) ^ 4 0C/min -> 60 0C (5 min) ^ 8 0C/min -

> 250 0C (3 min); CAS no: 96764; Active phase: HP-Innowax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Viegas, M. C.; Bassoli, D. G., Utilizacao do indice de retencao linear para caracterizacao de compostos volateis em cafe soluvel utilizando GC-MS e coluna HP-Innowax, Quim. Nova, 30(8), 2007, 2031-2034.)NIST Spectranist ri

2321 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 60 m;

Column type: Capillary; CAS no: 96764; Active phase: HP-Innowax; Carrier gas: Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Viegas, M. C.; Bassoli, D. G., Utilizacao do indice de retencao linear para caracterizacao de compostos volateis em cafe soluvel utilizando GC-MS e coluna HP-Innowax, Quim. Nova, 30(8), 2007, 2031-2034.)NIST Spectranist ri

- **Retention Index (Linear):**

  1539 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column length: 2 m;

Column type: Packed;

Heat rate: 4 K/min;

Start T: 80 C; End T:

250 C; CAS no: 96764;

Active phase: SE-30;

Substrate: GasChrom

Q; Data type: Linear RI;

Authors: Staniewski, J.,

Gas chromatographic

analysis of some

hydroxyoxime

extractants of metals,

Chem. Anal. (Warsaw),

36(2), 1991, 325-

333.)NIST Spectranist ri

1513 (Program type:

Ramp; Column cl…

(show more)ass: Semi-

standard non-polar;

Column diameter: 0. 25

mm; Column length: 30

m; Column type:

Capillary; Heat rate: 4

K/min; Start T: 80 C;

End T: 300 C; CAS no:

96764; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Zhao C. X.; Li, X. N.; Liang Y. Z.; Fang H. Z.; Huang L. F.; Guo F. Q., Comparative analysis of chemical components of essential oils from different samples of Rhododendron with the help of chemometrics methods, Chemom. Intell. Lab. Syst., 82, 2006, 218-228.)NIST Spectranist ri

1512 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30

m; Column type:
Capillary; Heat rate: 3
K/min; Start T: 60 C;
End T: 240 C; CAS no:
96764; Active phase:
DB-5; Carrier gas: H2;
Phase thickness: 0. 25
um; Data type: Linear
RI; Authors: Nogueira,
P. C. L.; Bittrich, V.;
Shepherd, G. J.; Lopes,
A. V.; Marsaioli, A. J.,
The ecological and
taxonomic importance
of flower volatiles of
Clusia species
(Guttiferae),
Phytochemistry, 56,
2001, 443-452.)NIST
Spectranist ri

2280 (Program type:
Ramp; Column cl...
(show more)ass:
Standard polar; Column
diameter: 0. 32 mm;

Column length: 50 m;

Column type: Capillary;

Heat rate: 4 K/min;

Start T: 60 C; End T:

220 C; End time: 30

min; Start time: 5 min;

CAS no: 96764; Active

phase: CP-Wax 52CB;

Data type: Linear RI;

Authors: Mahadevan,

K.; Farmer, L., Key

Odor Impact

Compounds in Three

Yeast Extract Pastes, J.

Agric. Food Chem., 54,

2006, 7242-7250.)NIST

Spectranist ri

2327 (Program type:

Ramp; Column cl…

(show more)ass:

Standard polar; Column

diameter: 0. 25 mm;

Column length: 60 m;

Column type: Capillary;

Heat rate: 3 K/min;

Start T: 40 C; End T: 240 C; End time: 10 min; Start time: 5 min; CAS no: 96764; Active phase: Stabilwax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Cros, S.; Lignot, B.; Bourseau, P.; Jaouen, P.; Prost, C., Desalination of mussel cooking juices by electrodialysis: effect on the aroma profile, J. Food Eng., 69, 2005, 425-436., Program type: Ramp; Column cl... (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 40 C; End T: 240 C; End time: 10

min; Start time: 5 min;

CAS no: 96764; Active

phase: Stabilwax;

Carrier gas: He; Phase

thickness: 0. 25 um;

Data type: Linear RI;

Authors: Cros, S.;

Vandanjon, L.; Jaouen,

P.; Bourseau, P.,

Processing of industrial

mussel cooking juices

by reverse osmosis:

pollution abatement

and aromas recovery,

2003.)NIST Spectranist

ri

2316 (Program type:

Ramp; Column cl…

(show more)ass:

Standard polar; Column

diameter: 0. 25 mm;

Column length: 60 m;

Column type: Capillary;

Heat rate: 2 K/min;

Start T: 35 C; End T:

195 C; End time: 90 min; Start time: 5 min; CAS no: 96764; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Chung, H. Y.; Yung, I. K. S.; Kim, J.-S., Comparison of volatile components in dried scallops (Chlamys farreri and Patinopecten yessoensis) prepared by boiling and steaming methods, J. Agric. Food Chem., 49, 2001, 192-202., Program type: Ramp; Column cl... (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary;

Heat rate: 2 K/min;

Start T: 35 C; End T:

195 C; End time: 90

min; Start time: 5 min;

CAS no: 96764; Active

phase: Supelcowax-10;

Carrier gas: He; Phase

thickness: 0. 25 um;

Data type: Linear RI;

Authors: Chung, H.-Y.;

Yung, I. K. S.; Ma, W. C.

J.; Kim, J.-S., Analysis of

volatile components in

frozen and dried

scallops (Patinopecten

yessoensis) by gas

chromatography/mass

spectrometry, Food

Res. Int., 35, 2002, 43-

53.)NIST Spectranist ri

2317 (Program type:

Ramp; Column cl…

(show more)ass:

Standard polar; Column

diameter: 0. 25 mm;

Column length: 60 m;

Column type: Capillary;

Heat rate: 2 K/min;

Start T: 35 C; End T:

195 C; End time: 90

min; Start time: 5 min;

CAS no: 96764; Active

phase: Supelcowax-10;

Carrier gas: He; Phase

thickness: 0. 25 um;

Data type: Linear RI;

Authors: Chung, H. Y.,

Volatile components in

crabmeats of Charybdis

feriatus, J. Agric. Food

Chem., 47, 1999, 2280-

2287.)NIST Spectranist

ri

2321 (Program type:

Ramp; Column cl…

(show more)ass:

Standard polar; Column

diameter: 0. 25 mm;

Column length: 60 m;

Column type: Capillary;

Heat rate: 2 K/min;

Start T: 50 C; End T:

230 C; End time: 60

min; CAS no: 96764;

Active phase: DB-Wax;

Carrier gas: He; Phase

thickness: 0. 25 um;

Data type: Linear RI;

Authors: Shiratsuchi,

H.; Shimoda, M.;

Imayoshi, K.; Noda, K.;

Osajima, Y., Volatile

flavor compounds in

spray-dried skim milk

powder, J. Agric. Food

Chem., 42, 1994, 984-

988.)NIST Spectranist ri

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

Density:	0. 9±0. 1 g/cm ^{3}
Boiling Point:	265. 5±9. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 6 mmHg at 25°C
Enthalpy of Vaporization:	52. 4±3. 0 kJ/mol

Flash Point:	115. 0±0. 0 °C
Index of Refraction:	1. 499
Molar Refractivity:	64. 9±0. 3 cm^3
#H bond acceptors:	1
#H bond donors:	1
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0
ACD/LogP:	4. 86
ACD/LogD (pH 5. 5):	4. 72
ACD/BCF (pH 5. 5):	2279. 83
ACD/KOC (pH 5. 5):	8814. 20
ACD/LogD (pH 7. 4):	4. 72
ACD/BCF (pH 7. 4):	2279. 68
ACD/KOC (pH 7. 4):	8813. 59
Polar Surface Area:	20 $Å^2$

Polarizability: 25. 7±0. 5 10^{-24} cm^3

Surface Tension: 30. 1±3. 0 dyne/cm

Molar Volume: 221. 2±3. 0 cm^3

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

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 5. 33Log Kow (Exper. database match) = 5. 19Exper. Ref: Chem Inspect Test Inst (1992)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 281. 15 (Adapted Stein & Brown method)Melting Pt (deg C): 76. 96 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00267 (Modified Grain method)MP (exp database): 56. 5 deg CBP (exp database): 263. 5 deg CVP (exp database): 4. 77E-03 mm Hg at 25 deg CSubcooled liquid VP: 0. 00977 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): 5. 704log Kow used: 5. 19 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 35 mg/L (25 deg C)Exper. Ref: CHEM INSPECT TEST INST (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 32. 493 mg/LWat Sol (Exper. database match) = 35. 00Exper. Ref: CHEM INSPECT TEST INST (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: PhenolsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 3. 74E-006 atm-m3/moleGroup Method: 3. 15E-006 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 271E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 19 (exp database)Log Kaw used: -3. 816 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 9. 006Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 3973Biowin2 (Non-Linear Model) : 0. 0788Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 3753 (weeks-months)Biowin4 (Primary Survey Model) : 3. 2829 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3249Biowin6 (MITI Non-Linear Model): 0. 1588Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 5154Ready 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. 3 Pa (0. 00977 mm Hg)Log Koa (Koawin est): 9. 006Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 3E-006 Octanol/air (Koa) model: 0. 000249 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 8. 32E-005 Mackay model : 0. 000184 Octanol/air (Koa) model: 0. 0195 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 49. 1082 E-12 cm3/molecule-secHalf-Life = 0. 218 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 2. 614 HrsOzone Reaction: No Ozone Reaction EstimationReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 0. 000134 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 393E+004Log Koc: 4. 144 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 = 2. 846 (BCF = 701. 9)log Kow used: 5. 19 (expkow database)Volatilization from Water: Henry LC: 3. 15E-006 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 268. 4 hours (11. 19 days)Half-Life from Model Lake : 3049 hours (127 days)Removal In Wastewater Treatment: Total removal: 82. 89 percentTotal biodegradation: 0. 71 percentTotal sludge adsorption: 82. 16 percentTotal to Air: 0. 02 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 151 5. 23 1000 Water 9. 94 900 1000 Soil 55. 8 1. 8e+003 1000 Sediment 34. 1 8. 1e+003 0 Persistence Time: 1. 56e+003 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop