Tcep c6h12cl3o4p structure

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Contents

Molecular Formula	$C_6H_{12}Cl_3O_4P$
Average mass	285. 490 Da
Density	1. 4±0. 1 g/cm ^{3}
Boiling Point	347. 4±0. 0 °C at 760 mmHg
Flash Point	232. 2±0. 0 °C

Molar Refractivity	56. 5±0. 3 cm^3
Polarizability	22. 4±0. 5 10^{-24} cm^3
Surface Tension	40. 6±3. 0 dyne/cm
Molar Volume	205. 0±3. 0 cm^3

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite
- Predicted – ChemAxon
- Experimental Physico-chemical Properties
  - **Experimental Melting Point:**

    -55 °CJean-Claude

    Bradley Open Melting

    Point Dataset20311

    -51

    °CLabNetworkLN00200

    312
  - **Experimental Flash Point:**

    222

°CLabNetworkLN00200

312

- Miscellaneous

  - **Safety:**

    IRRITANTMatrix

    Scientific098551

  - **Target Organs:**

    OthersTargetMolT0

    653

  - **Bio Activity:**

    OthersTargetMolT0

    653

- Gas Chromatography

  - **Retention Index (Kovats):**

    1740 (Program type:

    Isothermal; Col… (show

    more)umn class:

    Standard non-polar;

    Column length: 1. 5 m;

    Column type: Packed;

    CAS no: 115968; Active

    phase: SE-30; Carrier

gas: He; Substrate: Chromosorb G HP (80-100 mesh); Data type: Kovats RI; Authors: Ramsey, J. D.; Lee, T. D.; Osselton, M. D.; Moffat, A. C., Gas-liquid chromatographic retention indices of 296 non-drug substances on SE-30 or OV-1 likely to be encountered in toxicological analyses, J. Chromatogr., 184, 1980, 185-206.)NIST Spectranist ri

- **Retention Index (Lee):**

295. 96 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 115968; Active phase: Methyl Silicone; Data type: Lee RI;

Authors: Eckel, W. P.; Ross, B.; Isensee, R. K., Pentobarbital found in ground water, Ground Water, 31(5), 1993, 801-804.)NIST Spectranist ri

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

  1740 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Other; CAS no: 115968; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J.

Chromatogr., 220,

1981, 195-252.)NIST

Spectranist ri

1747. 2 (Program type:

Ramp; Column cl…

(show more)ass:

Standard non-polar;

Column diameter: 0. 2

mm; Column length: 1.

8 m; Column type:

Packed; Heat rate: 8

K/min; Start T: 150 C;

End T: 230 C; End time:

10 min; Start time: 2

min; CAS no: 115968;

Active phase: OV-101;

Carrier gas: He;

Substrate: Chromosorb

750; Data type: Normal

alkane RI; Authors:

LeBel, G. L.; Williams,

D. T.; Benoit, F. M., Gas

chromatographic

determination of

trialkyl/aryl phosphates

in drinking water, following isolation using macroreticular resin, J. Ass. Offic. Anal. Chem, 64(4), 1981, 991-998.)NIST Spectranist ri

- **Retention Index (Linear):**

  1776 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 115968; Active phase: HP-5MS; Data type: Linear RI; Authors: Hankemeier, Th.; Rozenbrand, J.; Abhadur, M.; Vreuls, J. J.; Brinkman, U. A. Th., Data Correlation in On-Line Solid-Phase Extraction – Gas Chromatography – Atomic Emission / Mass

Spectrometric
Detection of Unknown
Microcontaminants,
Chromatographia,
48(3/4), 1998, 273-
283.)NIST Spectranist ri

1777 (Program type:
Ramp; Column cl…
(show more)ass: Semi-
standard non-polar;
Column type: Capillary;
CAS no: 115968; Active
phase: HP-5MS; Data
type: Linear RI;
Authors: Hankemeier,
Th.; Rozenbrand, J.;
Abhadur, M.; Vreuls, J.
J.; Brinkman, U. A. Th.,
Data Correlation in On-
Line Solid-Phase
Extraction – Gas
Chromatography –
Atomic Emission / Mass
Spectrometric
Detection of Unknown

Microcontaminants, Chromatographia, 48(3/4), 1998, 273-283.)NIST Spectranist ri

1781 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 115968; Active phase: HP-5MS; Data type: Linear RI; Authors: Hankemeier, Th.; Rozenbrand, J.; Abhadur, M.; Vreuls, J. J.; Brinkman, U. A. Th., Data Correlation in On-Line Solid-Phase Extraction – Gas Chromatography – Atomic Emission / Mass Spectrometric Detection of Unknown Microcontaminants, Chromatographia,

48(3/4), 1998, 273-

283.)NIST Spectranist ri

1782 (Program type:

Ramp; Column cl…

(show more)ass: Semi-

standard non-polar;

Column type: Capillary;

CAS no: 115968; Active

phase: HP-5MS; Data

type: Linear RI;

Authors: Hankemeier,

Th.; Rozenbrand, J.;

Abhadur, M.; Vreuls, J.

J.; Brinkman, U. A. Th.,

Data Correlation in On-

Line Solid-Phase

Extraction – Gas

Chromatography –

Atomic Emission / Mass

Spectrometric

Detection of Unknown

Microcontaminants,

Chromatographia,

48(3/4), 1998, 273-

283.)NIST Spectranist ri

1766 (Program type:

Complex; Column...

(show more)class:

Semi-standard non-

polar; Column

diameter: 0. 31 mm;

Column length: 25 m;

Column type: Capillary;

Description:

50C(2min)=>(20C/min)

=>

120C=>(7C/min)=>

310C(10min); CAS no:

115968; Active phase:

5 % Phenyl methyl

siloxane; Carrier gas:

He; Phase thickness: 0.

52 um; Data type:

Linear RI; Authors:

Yasuhara, A.; Shiraishi,

H.; Nishikawa, M.;

Yamamoto, T.; Uehiro,

T.; Nakasugi, O.;

Okumura, T.;

Kenmotsu, K.; Fukui,

H.; Nagase, M.; Ono, Y.;

Kawagoshi, Y.; Baba, K.; Noma, Y., Determination of organic components in leachates from hazardous waste disposal sites in Japan by gas chromatography-mass spectrometry, J. Chromatogr. A, 774, 1997, 321-332.)NIST Spectranist ri

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

Density:	1. 4±0. 1 g/cm ^{3}
Boiling Point:	347. 4±0. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 7 mmHg at 25°C
Enthalpy of Vaporization:	56. 8±3. 0 kJ/mol
Flash Point:	232. 2±0. 0 °C
Index of Refraction:	1. 463

Molar Refractivity:	56. 5±0. 3 cm^{3}
#H bond acceptors:	4
#H bond donors:	0
#Freely Rotating Bonds:	9
#Rule of 5 Violations:	0
ACD/LogP:	0. 48
ACD/LogD (pH 5. 5):	1. 42
ACD/BCF (pH 5. 5):	7. 05
ACD/KOC (pH 5. 5):	140. 88
ACD/LogD (pH 7. 4):	1. 42
ACD/BCF (pH 7. 4):	7. 05
ACD/KOC (pH 7. 4):	140. 88
Polar Surface Area:	55 $Å^{2}$
Polarizability:	22. 4±0. 5 10^{-24} cm^{3}
Surface Tension:	40. 6±3. 0 dyne/cm

Molar Volume: 205. 0±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) = 1. 63Log Kow (Exper. database match) = 1. 44Exper. Ref: Chem Inspect Test Inst (1992)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 351. 67 (Adapted Stein & Brown method)Melting Pt (deg C): 82. 99 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 000391 (Modified Grain method)MP (exp database): -35 deg CBP (exp database): 330 deg CVP (exp database): 6. 13E-02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 877. 9log Kow used: 1. 44 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 7000 mg/L (deg C)Exper. Ref: MUIR, DCG (1984)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 5596. 7 mg/LWat Sol (Exper. database match) = 7000. 00Exper. Ref: MUIR, DCG (1984)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersEsters (phosphate)Henrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 55E-008 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 673E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 44 (exp database)Log Kaw used: -5. 982 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 422Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5914Biowin2 (Non-Linear Model) : 1. 0000Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 2025 (months)Biowin4 (Primary Survey Model) : 3. 5994 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3173Biowin6 (MITI Non-Linear Model): 0. 0193Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 4751Ready 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): 8. 17 Pa (0. 0613 mm Hg)Log Koa (Koawin est): 7. 422Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 67E-007 Octanol/air (Koa) model: 6. 49E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 33E-005 Mackay model : 2. 94E-005 Octanol/air (Koa) model: 0. 000519 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 21. 9884 E-12 cm3/molecule-secHalf-Life = 0. 486 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 5. 837 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 13E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 300. 9Log Koc: 2. 478 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. 371 (BCF = 0. 4254)log Kow used: 1. 44 (expkow database)Volatilization from Water: Henry LC: 2. 55E-008 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 3. 88E+004 hours (1617 days)Half-Life from Model Lake : 4. 234E+005 hours (1. 764E+004 days)Removal In Wastewater Treatment: Total removal: 1. 96 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 86 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. 176 11. 7 1000 Water

38. 2 1. 44e+003 1000 Soil 61. 5 2. 88e+003 1000 Sediment 0. 095 1. 3e+004 0
Persistence Time: 1. 2e+003 hr

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