

# [Tcep c6h12cl3o4p structure](https://assignbuster.com/tcep-c6h12cl3o4p-structure/)

\n[toc title="Table of Contents"]\n

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1. [Experimental Melting Point:](#experimental-melting-point) \n \t
2. [Experimental Flash Point:](#experimental-flash-point) \n \t
3. [Safety:](#safety) \n \t
4. [Target Organs:](#target-organs) \n \t
5. [Bio Activity:](#bio-activity) \n \t
6. [Retention Index (Kovats):](#retention-index-kovats) \n \t
7. [Retention Index (Lee):](#retention-index-lee) \n \t
8. [Retention Index (Normal Alkane):](#retention-index-normal-alkane) \n \t
9. [Retention Index (Linear):](#retention-index-linear) \n

\n[/toc]\n \n

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 6 H 12 Cl 3 O 4 P |
| 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 °CLabNetworkLN00200312 |

## Experimental Flash Point:

|  |
| --- |
| 222 °CLabNetworkLN00200312 |

* Miscellaneous

## Safety:

|  |
| --- |
| IRRITANTMatrix Scientific098551 |

## Target Organs:

|  |
| --- |
| OthersTargetMolT0653 |

## Bio Activity:

|  |
| --- |
| OthersTargetMolT0653 |

* 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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