

Dichlorfenthion
c10h13cl2o3ps
structure



Contents

- Retention Index (Linear):

Molecular
Formula $C_{10}H_{13}Cl_2O_3PS$

Average mass 315. 153 Da

Density $1.4 \pm 0.1 \text{ g/cm}^3$

Boiling Point $345.5 \pm 52.0 \text{ }^\circ\text{C}$ at 760
mmHg

Flash Point $162.7 \pm 30.7 \text{ }^\circ\text{C}$

Molar
Refractivity $74.2 \pm 0.3 \text{ cm}^3$

Polarizability $29.4 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$

Surface Tension $47.5 \pm 3.0 \text{ dyne/cm}$

Molar Volume $231.6 \pm 3.0 \text{ cm}^3$

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite
- Predicted - ChemAxon
- Gas Chromatography

- **Retention Index (Kovats):**

1852 (Program type: Isothermal; Col... (show more)umn class: Standard polar; Column diameter: 0. 53 mm; Column type: Packed; Start T: 210 C; 97176; Active phase: SE-30; Carrier gas: N2; Substrate: AW-DMCS; Data Kovats RI; Authors: Oyama, N.; Sano, T.; Syoyama, M.; Maeda, K., Studies systematic analysis of poisonous compounds in forensic chemistry. II. Ap of capillary column gas chromatography to substance identification by m retention indices, Eisei Kagaku, 33(5), 1987, 342-348.)NIST Spectranist r

1869 (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) 97176; 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

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

1843. 2 (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: 97176; 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

1821 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 97176; Active phase: Ultra-1; Data type: Normal alkane RI; Authors: Tameo, O.; Kiyos, I., Simultaneous determination of pesticides by capillary gas chromatography, Cannot be traslated (in Japan), 14(2), 1977, 109-122.)NIST Spectranist ri

1832. 7 (Program type: Complex; Column... (show more)class: Standard non-polar; Column diameter: 0. 2 mm; Column length: 25 m; Column type: Capillary; Description: 1 min at 100 0C; 100 - 150 0C at 30 deg/min; 2 min at 150 0C; 150 - 205 0C at 3 deg/min; 205 - 240 0C at 10 deg/min; 240 - 260 0C at 2 deg/min at 260 0C; CAS no: 97176; Active phase: HP-1; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Stan, H.-J., Application of Capillary Gas Chromatography with Mass Selective Detection to Pesticide Residue Analysis, J. Chromatogr., 467, 1989, 85-98.)NIST Spectranist ri

1849. 7 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column length: 1. 1 m; Column type: Packed; Heat rate: 8. 5 K/min; Start T: 100 C; End T: 300 C; CAS no: 97176; Active phase: OV-101; Carrier gas: N2; Substrate: Chromosorb W HP; Data type: Normal alkane RI; Authors: Saxton, W. L., Emergence temperature indices and relative retention times of pesticides and industrial chemicals determined by linear programmed temperature gas chromatography, J. Chromatogr., 393, 1987, 175-194.)NIST Spectranist ri

1835 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column length: 1 m; Column type: Packed; Heat rate: 4 K/min; Start T: 100 C; End T: 300 C; CAS no: 97176; Active phase: OV-101; Carrier gas: N2; Substrate: Chromosorb W HP; Data type: Normal alkane RI; Authors: Saxton, W. L., Emergence temperature indices and relative retention times of pesticides and industrial chemicals determined by linear programmed temperature gas chromatography, J. Chromatogr., 393, 1987, 175-194.)NIST Spectranist ri

End T: 210 C; End time: 20 min; CAS no: 97176; Active phase: OV-1; Carrier gas: Helium; Substrate: Chromosorb W AW DMCS; Data type: Normal alkane RI; Authors: TSunoda, N., Simultaneous determination of organophosphorous pesticides in forensic chemistry by gas-liquid chromatography with hydrogen flame ionization detector, Eisei Kagaku, 32(2), 1986, 91-100.)NIST Spectra

1850 (Program type: Isothermal; Column class: Standard non-polar; Column length: 1 m; Column type: Packed; Start T: 190 C; CAS no: 97176; Active phase: OV-1; Carrier gas: Helium; Substrate: Chromosorb W AW DMCS; Data type: Normal alkane RI; Authors: TSunoda, N., Simultaneous determination of organophosphorous pesticides in forensic chemistry by gas-liquid chromatography with hydrogen flame ionization detector, Eisei Kagaku, 32(2), 1986, 91-100.)NIST Spectra

1848. 4 (Program type: Complex; Column 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: 97176; 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 Spectra

1855. 2 (Program type: Ramp; Column class: Standard non-polar; Column type: Packed; Heat rate: 4 K/min; Start T: 200 C; End T: 290 C; CAS no: 97176; Active phase: OV-1; Carrier gas: Helium; Substrate: Chromosorb W AW DMCS; Data type: Normal alkane RI; Authors: TSunoda, N., Simultaneous determination of organophosphorous pesticides in forensic chemistry by gas-liquid chromatography with hydrogen flame ionization detector, Eisei Kagaku, 32(2), 1986, 91-100.)NIST Spectra

97176; Active phase: SE-30; Data type: Normal alkane RI; Authors: Krijgs W.; van de Kamp, C. G., Analysis of organophosphorus pesticides by capillary chromatography with flame photometric detection, J. Chromatogr., 117, 201-205.)NIST Spectranist ri

1845. 4 (Program type: Ramp; Column cl... (show more)ass: Standard non-polar; Column length: 2. 4 m; Column type: Packed; Heat rate: 10 K/min; Start T: 50 C; End T: 300 C; CAS no: 97176; Active phase: OV-101; Substrate: Gas Chromatography; Data type: Normal alkane RI; Authors: Bowman, M. C.; Beroza, M., GLC Residuals of Pesticides and Metabolites Containing Phosphorus and Sulfur on Thermally Stable Columns, J. Ass. Offic. Anal. Chem, 53(3), 1970, 499-500.)NIST Spectranist ri

1873 (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(1 min) ^ 25 0C/min -> 125 0C ^ 10 0C/min -> 300 0C(1 min); CAS no: 97176; 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

1857. 4 (Program type: Complex; Column... (show more)class: Semi-standard non-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: 97176; Active phase: DB-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI;

Chu, X.-G.; Hu, X.-Z.; Yao, H.-Y., Determination of 266 pesticide residues in orange juice by matrix solid-phase dispersion and gas chromatography-mass spectrometry detection, J. Chromatogr. A, 1063, 2005, 201-210.)NIST Spectranist ri

1869 (Program type: Complex; Column... (show more)class: Semi-standard; Column type: Non-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 (1 min); CAS no: 97176; 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), 2005, 1440-1451.)NIST Spectranist ri

1866. 3 (Program type: Complex; Column... (show more)class: Semi-standard; Column type: Non-polar; Column diameter: 0.2 mm; Column length: 25 m; Column type: Capillary; Description: 100C(1min) => 30C/min=> 150C(2min) => 3C/min=> 205C => 10C/min => 260C(29min); CAS no: 97176; Active phase: SE-54; Phase thickness: 0.33 um; Data type: Normal alkane RI; Authors: Stan, H.-J., Pesticide residue analysis in foodstuffs applying capillary gas chromatography with mass spectrometric detection State-of-the-art use of modified DFG-multimethods and automated data evaluation, J. Chromatogr. A, 892, 2000, 347-377.)NIST Spectranist ri

2576 (Program type: Ramp; Column cl... (show more)ass: Standard polar; Column type: Capillary; CAS no: 97176; Active phase: Carbowax 20M; Data type: Normal alkane RI; Authors: Tameo, O.; Kiyos, I., Simultaneous determination of pesticides in orange juice by capillary gas chromatography, Cannot be translated (in Japan), 14(2), 1991, 101-106.)NIST Spectranist ri

109-122.)NIST Spectranist ri

- **Retention Index (Linear):**

1820 (Program type: Ramp; Column cl... (show more)ass: Standard non-p

Column diameter: 0. 53 mm; Column length: 12 m; Column type: Capilla

rate: 6 K/min; Start T: 120 C; End T: 250 C; CAS no: 97176; Active phase:

Carrier gas: N2; Data type: Linear RI; Authors: Oyama, N.; Sano, T.; Syoy

Maeda, K., Studies on systematic analysis of poisonous compounds in for

chemistry. II. Application of capillary column gas chromatography to sub

identification by means of retention indices, Eisei Kagaku, 33(5), 1987, 3

348.)NIST Spectranist ri

1822 (Program type: Ramp; Column cl... (show more)ass: Standard non-p

Column diameter: 0. 53 mm; Column type: Packed; Heat rate: 2 K/min; S

80 C; End T: 220 C; CAS no: 97176; Active phase: OV-1; Carrier gas: N2;

Substrate: AW-DMCS; Data type: Linear RI; Authors: Oyama, N.; Sano, T.;

Syoyama, M.; Maeda, K., Studies on systematic analysis of poisonous cor

in forensic chemistry. II. Application of capillary column gas chromatogra

substance identification by means of retention indices, Eisei Kagaku, 33(

342-348.)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: 345. 5±52. 0 °C at 760 mmHg

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Vapour Pressure:	0. 0±0. 7 mmHg at 25°C
Enthalpy of Vaporization:	56. 6±3. 0 kJ/mol
Flash Point:	162. 7±30. 7 °C
Index of Refraction:	1. 554
Molar Refractivity:	74. 2±0. 3 cm ³
#H bond acceptors:	3
#H bond donors:	0
#Freely Rotating Bonds:	6
#Rule of 5 Violations:	1
ACD/LogP:	5. 12
ACD/LogD (pH 5. 5):	4. 88
ACD/BCF (pH 5. 5):	2991. 62
ACD/KOC (pH 5. 5):	10706. 53
ACD/LogD (pH 7. 4):	4. 88
ACD/BCF (pH 7. 4):	2991. 62

ACD/KOC (pH 7. 4):	10706. 53
Polar Surface Area:	70 Å ²
Polarizability:	29. 4±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	47. 5±3. 0 dyne/cm
Molar Volume:	231. 6±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. 20Log Kow (Exper. database match) = 5. 14Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 353. 30 (Adapted Stein & Brown method)Melting Pt (deg C): 32. 87 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 9. 37E-005 (Modified Grain method)BP (exp database): 164-169 @ 0. 1 mm Hg deg CVP (exp database): 5. 60E-04 mm Hg at 25 deg CSubcooled liquid VP: 0. 00067 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): 0. 408log Kow used: 5. 14 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 0. 245 mg/L (25 deg C)Exper. Ref: CHIOU, CT ET AL. (1977)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 93351 mg/LWat Sol (Exper. database match) = 0. 25Exper. Ref: CHIOU, CT ET AL. (1977)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersEsters (phosphate)Nearest analog analysis: pesticidesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 4. 12E-005 atm-m³/moleGroup Method: IncompleteExper Database: 9. 48E-04 atm-m³/moleHenrys LC [VP/WSol estimate using EPI values]: 9. 523E-005 atm-m³/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 14 (exp database)Log Kaw used: -1. 412 (exp database)Log Koa (KOAWIN v1. 10 estimate): 6. 552Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5466Biowin2 (Non-Linear Model) : 1. 0000Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 2433 (months)Biowin4 (Primary Survey Model) : 3. 5277 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 0659Biowin6 (MITI Non-Linear Model): 0. 0097Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 1651Ready 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): 0. 0893 Pa (0. 00067 mm Hg)Log Koa (Koawin est): 6. 552Kp (particle/gas partition coef. (m³/ug)): Mackay model : 3. 36E-005 Octanol/air (Koa) model: 8. 75E-007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 00121 Mackay model : 0. 00268 Octanol/air (Koa) model: 7E-005 Atmospheric Oxidation (25 deg C) [AopWin v1.

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92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 92. 3373 E-12
cm³/molecule-secHalf-Life = 0. 116 Days (12-hr day; 1. 5E6 OH/cm³)Half-Life =
1. 390 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to
airborne particulates (phi): 0. 00195 (Junge, Mackay)Note: the sorbed
fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient
(PCKOCWIN v1. 66): Koc : 4131Log Koc: 3. 616 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 = 3. 258 (BCF = 1811)log Kow used: 5. 14
(expkow database)Volatilization from Water: Henry LC: 0. 000948 atm-m³/mole
(Henry experimental database)Half-Life from Model River: 2. 908 hoursHalf-
Life from Model Lake : 180. 6 hours (7. 524 days)Removal In Wastewater
Treatment: Total removal: 83. 39 percentTotal biodegradation: 0. 65
percentTotal sludge adsorption: 78. 07 percentTotal to Air: 4. 66
percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount
Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 106 2. 78 1000 Water 5. 02 1.
44e+003 1000 Soil 74. 2 2. 88e+003 1000 Sediment 20. 7 1. 3e+004 0
Persistence Time: 1. 85e+003 hr

[Click to predict properties on the Chemicalize site](https://assignbuster.com/dichlorfenthion-c10h13cl2o3ps-structure/)