

# [Propachlor c11h14clno structure](https://assignbuster.com/propachlor-c11h14clno-structure/)

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* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 11 H 14 ClNO  |
| Average mass  | 211. 688 Da  |
| Density  | 1. 1±0. 1 g/cm 3  |
| Boiling Point  | 290. 4±23. 0 °C at 760 mmHg  |
| Flash Point  | 129. 4±22. 6 °C  |
| Molar Refractivity  | 59. 3±0. 3 cm 3  |
| Polarizability  | 23. 5±0. 5 10 -24 cm 3  |
| Surface Tension  | 40. 8±3. 0 dyne/cm  |
| Molar Volume  | 185. 8±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Predicted – Mcule
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| 77 °CJean-Claude Bradley Open Melting Point Dataset21600  |

* Miscellaneous

## Therapeutical Effect:

|  |
| --- |
| herbicideMicrosource[00330052]  |

## Compound Source:

|  |
| --- |
| syntheticMicrosource[00330052]  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1553 (estimated with error: 89)NIST Spectramainlib\_125590, replib\_52384, replib\_53678, replib\_334578, replib\_378644  |
| 1608 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 15 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; End T: 270 C; CAS no: 1918167; Active phase: DB-1; Carrier gas: He; Data type: Kovats RI; Authors: Hall, G. L.; Whitehead, W. E.; Mourer, C. R.; Shibamoto, T., A new gas chromatographic retention index for pesticides and related compounds, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 9, 1986, 266-271.)NIST Spectranist ri  |
| 1617 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 15 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; End T: 270 C; CAS no: 1918167; Active phase: DB-5; Carrier gas: He; Data type: Kovats RI; Authors: Hall, G. L.; Whitehead, W. E.; Mourer, C. R.; Shibamoto, T., A new gas chromatographic retention index for pesticides and related compounds, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 9, 1986, 266-271.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1607. 5 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 55 C; End T: 210 C; End time: 30 min; Start time: 2 min; CAS no: 1918167; Active phase: DB-1; Data type: Normal alkane RI; Authors: Albanis, T. A.; Hela, D. G., Multi-residue pesticide analysis in environmental water samples using solid-phase extraction discs and gas chromatography with flame thermionic and mass-selective detection, J. Chromatogr. A, 707, 1995, 283-292.)NIST Spectranist ri  |
| 1612. 1 (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; 1 min at 260 0C; CAS no: 1918167; 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  |
| 1585. 8 (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: 50 C; End T: 300 C; CAS no: 1918167; 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  |
| 1585. 1 (Program type: Complex; Column… (show more)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 5 deg/min; hold at 250 C for elution of last component; CAS no: 1918167; 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 Spectranist ri  |
| 1585. 6 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 6 ft; Column type: Packed; CAS no: 1918167; Active phase: DC-200; Carrier gas: He; Substrate: Chromosorb W HP (80-100 mesh); Data type: Normal alkane RI; Authors: Laski, R. R.; Watts, R. R., Gas chromatography of organonitrogen pesticides, using a nitrogen-specific detection system, J. Ass. Offic. Anal. Chem, 55(2), 1973, 328-332.)NIST Spectranist ri  |
| 1612 (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 (10 min); CAS no: 1918167; 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 aadditives, and veterinary drugs in foods, 2006.)NIST Spectranist ri  |
| 1606. 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: 1918167; Active phase: DB-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Chu, X.-G.; Hu, X.-Z.; Yao, H.-Y., Determination of 266 pesticide residues in apple juice by matrix solid-phase dispersion and gas chromatography-mass selective detection, J. Chromatogr. A, 1063, 2005, 201-210.)NIST Spectranist ri  |
| 1605. 9 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 70C(2min) => 25C/min=> 150C=> 3C/min => 200C => 8C/min=> 280C(10min); CAS no: 1918167; Active phase: ZB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Albero, B.; Sanchez-Brunete, C.; Tadeo, J. L., Analysis of pesticides in honey by solid-phase extraction and gas chromatography-mass spectrometry, J. Agric. Food Chem., 52, 2004, 5828-5835.)NIST Spectranist ri  |
| 1620. 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: 70C(2min)=> 25C/min => 150C=> 3C/min => 200C => 8C/min=> 280C(10min); CAS no: 1918167; Active phase: ZB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Sanchez-Brunete, C.; Albero, B.; Tadeo, J. L., Multiresidue determination of pesticides in soil by gas chromatography-mass spectrometry detection, J. Agric. Food Chem., 52, 2004, 1445-1451.)NIST Spectranist ri  |
| 1595. 1 (Program type: Complex; Column… (show more)class: Semi-standard 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: 1918167; 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-multimethod S19 and automated data evaluation, J. Chromatogr. A, 892, 2000, 347-377.)NIST Spectranist ri  |
| 1577. 8 (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: 6 K/min; Start T: 60 C; End T: 260 C; End time: 12 min; CAS no: 1918167; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Mogadati, P.; Louis, J. B.; Rosen, J. D., Multiresidue determination of pesticides in high-organic-content soils by solid-phase extraction and gas chromatography/mass spectrometry, J. AOAC Int., 82(3), 1999, 705-715.)NIST Spectranist ri  |
| 1612. 5 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 150 C; End T: 275 C; End time: 3 min; Start time: 5 min; CAS no: 1918167; Active phase: RTX-5; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Normal alkane RI; Authors: Restek, Restek International, 1999 Product Guide, 1(1), 1999, 578-591, In original 578-591.)NIST Spectranist ri  |
| 1619. 6 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 100 C; End T: 275 C; End time: 2 min; Start time: 5 min; CAS no: 1918167; Active phase: RTX-5; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Normal alkane RI; Authors: Restek, Restek International, 1999 Product Guide, 1(1), 1999, 578-591, In original 578-591.)NIST Spectranist ri  |
| 1597 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 29 m; Column type: Capillary; Description: 80 C (1 min) ^ 6 C/min -> 200 C (3 min) ^ 6 C/min -> 260 C (8 min); CAS no: 1918167; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Papadopoulou-Mourkidou, E.; Patsias, J.; Kotopoulou, A., Determination of pesticides in soils by gas chromatography-ion trap mass spectrometry, J. AOAC Int., 80(2), 1997, 447-454.)NIST Spectranist ri  |
| 1608. 8 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 80(1)-6^ -> 200(3)-6^ -> 260(10); CAS no: 1918167; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Patsias, J.; Papadopoulou-Mourkidou, E., Rapid method for the analysis of a variety of chemical classes of pesticides in surface and ground waters by off-line solid phase extraction and gas chromatography-ion trap mass spectrometry, J. Chromatogr. A, 740, 1996, 83-98.)NIST Spectranist ri  |
| 1597. 6 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 75 0C (0. 67 min) ^ 10 0C/min -> 140 0C ^ 5 0C/min -> 250 0C (1 min) ^ 20 0C/min -> 320 0C (5 min); CAS no: 1918167; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Olson, N. L.; Carrell, R.; Cummings, R.; Rieck, R.; Reimer, S., Atomic emission detection for gas chromatographic analysis of nitrogen-containing herbicides in water, J. AOAC Int., 78(6), 1995, 1464-1473.)NIST Spectranist ri  |
| 1602. 8 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 57 0C (1 min) ^ 15 0C/min -> 130 0C (1 min) ^ 2. 3 0C/min -> 270 0C (20 min); CAS no: 1918167; Active phase: DB-5; Data type: Normal alkane RI; Authors: Bernal, J. L.; del Nozal, M. J.; Atienza, J.; Jimenez, J. J., Multidetermination of PCBs and pesticides by use of a dual GC column-dual detector system, Chromatographia, 33(1/2), 1992, 67-76.)NIST Spectranist ri  |
| 1616. 2 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: Capillary; Heat rate: 2. 8 K/min; Start T: 140 C; End T: 270 C; End time: 1 min; Start time: 2 min; CAS no: 1918167; Active phase: DB-5; Carrier gas: He; Phase thickness: 1. 5 um; Data type: Normal alkane RI; Authors: Lopez-Avila, V.; Benedicto, J.; Baldin, E.; Beckert, W. F., Analysis of classes of compounds of environmental concern: III. Organochlorine pesticides, J. Hi. Res. Chromatogr., 15, 1992, 319-328.)NIST Spectranist ri  |
| 2345 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column type: Capillary; CAS no: 1918167; Active phase: Carbowax 20M; 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), 1991, 109-122.)NIST Spectranist ri  |

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

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| --- | --- |
| Density:  | 1. 1±0. 1 g/cm 3  |
| Boiling Point:  | 290. 4±23. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 6 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 53. 0±3. 0 kJ/mol  |
| Flash Point:  | 129. 4±22. 6 °C  |
| Index of Refraction:  | 1. 551  |
| Molar Refractivity:  | 59. 3±0. 3 cm 3  |
| #H bond acceptors:  | 2  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 3  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 2. 28  |
| ACD/LogD (pH 5. 5):  | 2. 28  |
| ACD/BCF (pH 5. 5):  | 31. 89  |
| ACD/KOC (pH 5. 5):  | 414. 88  |
| ACD/LogD (pH 7. 4):  | 2. 28  |
| ACD/BCF (pH 7. 4):  | 31. 89  |
| ACD/KOC (pH 7. 4):  | 414. 89  |
| Polar Surface Area:  | 20 Å 2  |
| Polarizability:  | 23. 5±0. 5 10 -24 cm 3  |
| Surface Tension:  | 40. 8±3. 0 dyne/cm  |
| Molar Volume:  | 185. 8±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) = 2. 42Log Kow (Exper. database match) = 2. 18Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 322. 84 (Adapted Stein & Brown method)Melting Pt (deg C): 85. 56 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 000185 (Modified Grain method)MP (exp database): 77 deg CBP (exp database): 110 @ 0. 03 mm Hg deg CVP (exp database): 2. 30E-04 mm Hg at 25 deg CSubcooled liquid VP: 0. 000752 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): 523. 4log Kow used: 2. 18 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 700 mg/L (20 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1202. 5 mg/LWat Sol (Exper. database match) = 700. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: HaloacetamidesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 85E-008 atm-m3/moleGroup Method: IncompleteExper Database: 9. 15E-08 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 9. 845E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 18 (exp database)Log Kaw used: -5. 427 (exp database)Log Koa (KOAWIN v1. 10 estimate): 7. 607Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8736Biowin2 (Non-Linear Model) : 0. 9334Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5260 (weeks-months)Biowin4 (Primary Survey Model) : 3. 6520 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 2507Biowin6 (MITI Non-Linear Model): 0. 0855Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 3044Ready 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. 1 Pa (0. 000752 mm Hg)Log Koa (Koawin est ): 7. 607Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 99E-005 Octanol/air (Koa) model: 9. 93E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 00108 Mackay model : 0. 00239 Octanol/air (Koa) model: 0. 000794 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 20. 9713 E-12 cm3/molecule-secHalf-Life = 0. 510 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 6. 120 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 00173 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 284. 7Log Koc: 2. 454 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. 979 (BCF = 9. 519)log Kow used: 2. 18 (expkow database)Volatilization from Water: Henry LC: 9. 15E-008 atm-m3/mole (Henry experimental database)Half-Life from Model River: 9311 hours (388 days)Half-Life from Model Lake : 1. 017E+005 hours (4238 days)Removal In Wastewater Treatment: Total removal: 2. 45 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 35 percentTotal to Air: 0. 01 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 348 12. 2 1000 Water 24. 5 900 1000 Soil 75 1. 8e+003 1000 Sediment 0. 119 8. 1e+003 0 Persistence Time: 1. 05e+003 hr

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* 1-Click Scaffold Hop