Propachlor c11h14clno structure

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Contents

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[0033 0052]
  - **Compound Source:**

    syntheticMicrosource[0033 0052]
- Gas Chromatography

- **Retention Index (Kovats):**

  1553 (estimated with error: 89)NIST Spectramainlib_125590, replib_5238

  replib_53678, replib_334578, replib_378644

  1608 (Program type: Ramp; Column cl... (show more)ass: Standard non-p

  Column diameter: 0. 25 mm; Column length: 15 m; Column type: Capilla

  rate: 6 K/min; Start T: 100 C; End T: 270 C; CAS no: 1918167; Active pha

  Carrier gas: He; Data type: Kovats RI; Authors: Hall, G. L.; Whitehead, W.

  Mourer, C. R.; Shibamoto, T., A new gas chromatographic retention index

  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

  polar; Column diameter: 0. 25 mm; Column length: 15 m; Column type: C

  Heat rate: 6 K/min; Start T: 100 C; End T: 270 C; CAS no: 1918167; Active

  DB-5; Carrier gas: He; Data type: Kovats RI; Authors: Hall, G. L.; Whitehe

  E.; Mourer, C. R.; Shibamoto, T., A new gas chromatographic retention in

  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 no

  Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capilla

  rate: 5 K/min; Start T: 55 C; End T: 210 C; End time: 30 min; Start time: 2

  CAS no: 1918167; Active phase: DB-1; Data type: Normal alkane RI; Auth

  Albanis, T. A.; Hela, D. G., Multi-residue pesticide analysis in environmen

  samples using solid-phase extraction discs and gas chromatography with

thermionic and mass-selective detection, J. Chromatogr. A, 707, 1995, 28
292.)NIST Spectranist ri

1612. 1 (Program type: Complex; Column... (show more)class: Standard
polar; Column diameter: 0. 2 mm; Column length: 25 m; Column type: Ca
Description: 1 min at 100 0C; 100 – 150 0C at 30 deg/min; 2 min at 150 0
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: 1918167; Active phase: HP-1; Carrier gas: He; Ph
thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Stan, H.-J., Ap
of Capillary Gas Chromatography with Mass Selective Detection to Pestic
Residue Analysis, J. Chromatogr., 467, 1989, 85-98.)NIST Spectranist ri

1585. 8 (Program type: Ramp; Column cl... (show more)ass: Standard no
Column length: 1. 1 m; Column type: Packed; Heat rate: 8. 5 K/min; Start
End T: 300 C; CAS no: 1918167; Active phase: OV-101; Carrier gas: N2;
Substrate: Chromosorb W HP; Data type: Normal alkane RI; Authors: Sax
L., Emergence temperature indices and relative retention times of pestic
industrial chemicals determined by linear programmed temperature gas
chromatography, J. Chromatogr., 393, 1987, 175-194.)NIST Spectranist r

1585. 1 (Program type: Complex; Column... (show more)class: Standard
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
deg/min; hold at 250 C for elution of last component; CAS no: 1918167; A
phase: SE-30; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Nor
alkane RI; Authors: Ripley, B. D.; Braun, H. E., Retention time data for
organochlorine, organophosphorus, and organonitrogen pesticides on SE

capillary column and application of capillary gas chromatography to pest 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: Standa polar; Column length: 6 ft; Column type: Packed; CAS no: 1918167; Activ DC-200; Carrier gas: He; Substrate: Chromosorb W HP (80-100 mesh); Da Normal alkane RI; Authors: Laski, R. R.; Watts, R. R., Gas chromatograph organonitrogen pesticides, using a nitrogen-specific detection system, J. Offic. Anal. Chem, 55(2), 1973, 328-332.)NIST Spectranist ri

1612 (Program type: Complex; Column... (show more)class: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Description: 50 0C(1 min) ^ 25 0C/min -> 125 0C ^ 10 0C/min -> 300 0C min); CAS no: 1918167; Active phase: 5 % Phenyl methyl siloxane; Carrie Helium; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors Department of Food Safety, Ministry of Health; Welfare, Analytical metho residual compositional substances of agricultural chemicals, feed aadditi veterinary drugs in foods, 2006.)NIST Spectranist ri

1606. 4 (Program type: Complex; Column... (show more)class: Semi-stan non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty Capillary; Description: 80C(1min) => 10C/min => 160C (5min) => 3C/m 240C => 25C/min => 280C(10min); CAS no: 1918167; Active phase: DB 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 juice by matrix solid-phase dispersion and gas chromatography-mass sel

detection, J. Chromatogr. A, 1063, 2005, 201-210.)NIST Spectranist ri

1605. 9 (Program type: Complex; Column... (show more)class: Semi-stan non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty Capillary; Description: 70C(2min) => 25C/min=> 150C=> 3C/min => 20 8C/min=> 280C(10min); CAS no: 1918167; Active phase: ZB-5; Carrier g Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Albero, Sanchez-Brunete, C.; Tadeo, J. L., Analysis of pesticides in honey by solid extraction and gas chromatography-mass spectrometry, J. Agric. Food Ch 2004, 5828-5835.)NIST Spectranist ri

1620. 4 (Program type: Complex; Column... (show more)class: Semi-stan non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty Capillary; Description: 70C(2min)=> 25C/min => 150C=> 3C/min => 20 8C/min=> 280C(10min); CAS no: 1918167; Active phase: ZB-5; Carrier g Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Sanche Brunete, C.; Albero, B.; Tadeo, J. L., Multiresidue determination of pestici soil by gas chromatography-mass spectrometry detection, J. Agric. Food 52, 2004, 1445-1451.)NIST Spectranist ri

1595. 1 (Program type: Complex; Column... (show more)class: Semi-stan non-polar; Column diameter: 0. 2 mm; Column length: 25 m; Column typ Capillary; Description: 100C(1min) => 30C/min=> 150C(2min) => 3C/m 205C => 10C/min => 260C(29min); CAS no: 1918167; Active phase: SE- Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Stan, H Pesticide residue analysis in foodstuffs applying capillary gas chromatogr with mass spectrometric detection State-of-the-art use of modified DFG-

multimethod S19 and automated data evaluation, J. Chromatogr. A, 892, 347-377.)NIST Spectranist ri

1577. 8 (Program type: Ramp; Column cl... (show more)ass: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C 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 type: Normal alkane RI; Authors: Mogadati, P.; Louis, J. B.; Rosen, J. D., Multiresidue determination of pesticides in high-organic-content soils by phase extraction and gas chromatography/mass spectrometry, J. AOAC In 82(3), 1999, 705-715.)NIST Spectranist ri

1612. 5 (Program type: Ramp; Column cl... (show more)ass: Semi-standa polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: C Heat rate: 4 K/min; Start T: 150 C; End T: 275 C; End time: 3 min; Start ti min; CAS no: 1918167; Active phase: RTX-5; Carrier gas: He; Phase thick 5 um; Data type: Normal alkane RI; Authors: Restek, Restek Internationa Product Guide, 1(1), 1999, 578-591, In original 578-591.)NIST Spectranis

1619. 6 (Program type: Ramp; Column cl... (show more)ass: Semi-standa polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: C Heat rate: 4 K/min; Start T: 100 C; End T: 275 C; End time: 2 min; Start ti min; CAS no: 1918167; Active phase: RTX-5; Carrier gas: He; Phase thick 5 um; Data type: Normal alkane RI; Authors: Restek, Restek Internationa Product Guide, 1(1), 1999, 578-591, In original 578-591.)NIST Spectranis

1597 (Program type: Complex; Column... (show more)class: Semi-standa

polar; Column diameter: 0. 2 mm; Column length: 29 m; Column type: Ca

Description: 80 C (1 min) ^ 6 C/min -> 200 C (3 min) ^ 6 C/min -> 260 C

CAS no: 1918167; Active phase: DB-5; Carrier gas: He; Phase thickness:

um; Data type: Normal alkane RI; Authors: Papadopoulou-Mourkidou, E.;

J.; Kotopoulou, A., Determination of pesticides in soils by gas chromatogr

trap mass spectrometry, J. AOAC Int., 80(2), 1997, 447-454.)NIST Spectra

1608. 8 (Program type: Complex; Column... (show more)class: Semi-stan

non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty

Capillary; Description: 80(1)-6^ -> 200(3)-6^ -> 260(10); CAS no: 19181

Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data typ

Normal alkane RI; Authors: Patsias, J.; Papadopoulou-Mourkidou, E., Rapi

method for the analysis of a variety of chemical classes of pesticides in s

and ground waters by off-line solid phase extraction and gas chromatogr

trap mass spectrometry, J. Chromatogr. A, 740, 1996, 83-98.)NIST Spectr

1597. 6 (Program type: Complex; Column... (show more)class: Semi-stan

non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column ty

Capillary; Description: 75 0C (0. 67 min) ^ 10 0C/min -> 140 0C ^ 5 0C/

250 0C (1 min) ^ 20 0C/min -> 320 0C (5 min); CAS no: 1918167; Active

DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alka

Authors: Olson, N. L.; Carrell, R.; Cummings, R.; Rieck, R.; Reimer, S., Ato

emission detection for gas chromatographic analysis of nitrogen-containi

herbicides in water, J. AOAC Int., 78(6), 1995, 1464-1473.)NIST Spectrani

1602. 8 (Program type: Complex; Column... (show more)class: Semi-stan

non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column ty

Capillary; Description: 57 0C (1 min) ^ 15 0C/min -> 130 0C (1 min) ^ 2.
0C/min -> 270 0C (20 min); CAS no: 1918167; Active phase: DB-5; Data
Normal alkane RI; Authors: Bernal, J. L.; del Nozal, M. J.; Atienza, J.; Jimen
Multidetermination of PCBs and pesticides by use of a dual GC column-du
detector system, Chromatographia, 33(1/2), 1992, 67-76.)NIST Spectrani

1616. 2 (Program type: Ramp; Column cl... (show more)ass: Semi-standa
polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: C
Heat rate: 2. 8 K/min; Start T: 140 C; End T: 270 C; End time: 1 min; Star
min; CAS no: 1918167; Active phase: DB-5; Carrier gas: He; Phase thickn
um; Data type: Normal alkane RI; Authors: Lopez-Avila, V.; Benedicto, J.;
E.; Beckert, W. F., Analysis of classes of compounds of environmental co
Organochlorine pesticides, J. Hi. Res. Chromatogr., 15, 1992, 319-328.)NI
Spectranist ri

2345 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column type: Capillary; CAS no: 1918167; Active phase: Carbowax 20M;
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

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