

# [4,4′-dichlorobenzophenone c13h8cl2o structure](https://assignbuster.com/44-dichlorobenzophenone-c13h8cl2o-structure/)

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

\n \t

1. [Experimental Melting Point:](#experimental-melting-point) \n \t
2. [Experimental Boiling Point:](#experimental-boiling-point) \n \t
3. [Experimental LogP:](#experimental-logp) \n \t
4. [Experimental Flash Point:](#experimental-flash-point) \n \t
5. [Experimental Gravity:](#experimental-gravity) \n \t
6. [Predicted Melting Point:](#predicted-melting-point) \n \t
7. [Safety:](#safety) \n \t
8. [Retention Index (Kovats):](#retention-index-kovats) \n \t
9. [Retention Index (Normal Alkane):](#retention-index-normal-alkane) \n

\n[/toc]\n \n

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 13 H 8 Cl 2 O  |
| Average mass  | 251. 108 Da  |
| Density  | 1. 3±0. 1 g/cm 3  |
| Boiling Point  | 353. 0±0. 0 °C at 760 mmHg  |
| Flash Point  | 156. 2±24. 3 °C  |
| Molar Refractivity  | 65. 8±0. 3 cm 3  |
| Polarizability  | 26. 1±0. 5 10 -24 cm 3  |
| Surface Tension  | 46. 0±3. 0 dyne/cm  |
| Molar Volume  | 191. 4±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 147 °CTCID1621  |
| 144-146 °CAlfa Aesar  |
| 142-145 °CMerck Millipore4256, 841531  |
| 147. 5 °CJean-Claude Bradley Open Melting Point Dataset20954  |
| 145 °CJean-Claude Bradley Open Melting Point Dataset4407  |
| 144-146 °CAlfa AesarA12608  |
| 146-145 °CSynQuest2617-5-05  |
| 145 °CBiosynthW-100319  |
| 144-146 °CLabNetworkLN00206828  |
| 144-146 °CIndofine[CS-280]  |

## Experimental Boiling Point:

|  |
| --- |
| 352-354 °CAlfa AesarA12608  |
| 353 °CSynQuest2617-5-05  |
| 353 °CBiosynthW-100319  |
| 353 °CLabNetworkLN00206828  |

## Experimental LogP:

|  |
| --- |
| 4. 623Vitas-MSTK290986  |

## Experimental Flash Point:

|  |
| --- |
| 156 °CBiosynthW-100319  |
| 352-354 °CLabNetworkLN00206828  |

## Experimental Gravity:

|  |
| --- |
| 156 g/mLBiosynthW-100319  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 147 °CTCI  |
| 147 °CTCID1621  |

* Miscellaneous

## Safety:

|  |
| --- |
| 26-37Alfa AesarA12608  |
| 36/37/38Alfa AesarA12608  |
| H315-H319-H335Alfa AesarA12608  |
| IrritantSynQuest2617-5-05  |
| P261; P262BiosynthW-100319  |
| P261-P280-P305+P351+P338-P304+P340-P405-P501aAlfa AesarA12608  |
| WarningAlfa AesarA12608  |
| WARNING: Irritates lungs, eyes, skinAlfa AesarA12608  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1962 (estimated with error: 89)NIST Spectramainlib\_341065, replib\_59676, replib\_12161, replib\_235078  |
| 1947 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 190 C; CAS no: 90982; Active phase: OV-1; Data type: Kovats RI; Authors: Erdmann, F.; Rochholz, G.; Schutz, H., Retention-indices on OV-1 of approximately 170 commonly used pesticides, Mikrochim. Acta, 106, 1992, 219-226.)NIST Spectranist ri  |
| 1979 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 220 C; CAS no: 90982; Active phase: OV-1; Data type: Kovats RI; Authors: Erdmann, F.; Rochholz, G.; Schutz, H., Retention-indices on OV-1 of approximately 170 commonly used pesticides, Mikrochim. Acta, 106, 1992, 219-226.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1955. 1 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 2 mm; Column length: 12 m; Column type: Capillary; Heat rate: 18 K/min; Start T: 60 C; End T: 265 C; Start time: 1 min; CAS no: 90982; Active phase: HP-1; Carrier gas: He; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Liao, W.; Joe, T.; Cusick, W. G., Multiresidue screening method for fresh fruits and vegetables with gas chromatographic/mass spectrometric detection, J. Ass. Offic. Anal. Chem, 74(3), 1991, 554-565.)NIST Spectranist ri  |
| 2030 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 2 m; Column type: Packed; CAS no: 90982; Active phase: OV-101; Carrier gas: N2; Substrate: GAs Chrom Q (80-100 mesh); Data type: Normal alkane RI; Authors: Omura, M.; Hashimoto, K.; Ohta, K.; Iio, T.; Ueda, S.; Ando, K.; Fujiu, Y.; Hiraide, H., Effective application of the relative retention time diagram for gas chromatographic analysis of pesticides, J. Agric. Food Chem., 39(12), 1991, 2200-2205.)NIST Spectranist ri  |
| 1947. 1 (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: 90982; 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  |
| 1995. 8 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 6 ft; Column type: Packed; CAS no: 90982; Active phase: DC-200; Substrate: Chromosorb W (60-80 mesh); Data type: Normal alkane RI; Authors: Siewierski, M.; Helrich, K., Separation, identification, and measurement of DDT and its metabolites, J. Ass. Offic. Anal. Chem, 50(3), 1967, 627-633.)NIST Spectranist ri  |
| 2014 (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: 90982; 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  |
| 2018 (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: 90982; 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  |
| 1975. 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: 90982; Active phase: HP-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Wong, J. W.; Webster, M. G.; Bezabeh, D. Z.; Hengel, M. J.; Ngim, K. K.; Krynitsky, A. J.; Ebeler, S. E., Multiresidue determination of pesticides in malt beverages by capillary gas chromatography with mass spectrometry and selected ion monitoring, J. Agric. Food Chem., 52, 2004, 6361-6372.)NIST Spectranist ri  |
| 1971. 8 (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: 90982; 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  |
| 2015. 9 (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: 90982; 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  |
| 1980. 5 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Description: 90 0C (4 min) ^ 18 0C/min -; 180 0C (1 min) ^ 0. 9 0C/min -; 200 0C (1 min) ^ 1. 5 0C/min -; 270 0C (15 min); CAS no: 90982; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Najam, A. R.; Korver, M. P.; Williams, C. C.; Burse, V. W.; Needham, L. L., Analysis of a mixture of polychlorinated biphenyls and chlorinated pesticides in human serum by column fractionation and dual-column capillary gas chromatography with electron capture detection, J. AOAC Int., 82(1), 1999, 177-185.)NIST Spectranist ri  |
| 1980. 7 (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: 90982; 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  |
| 1989. 9 (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: 90982; 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  |
| 2008. 3 (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: 90982; 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  |
| 1973. 4 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 20 mm; Column length: 25 m; Column type: Capillary; Description: 90 0C (1 min) ^ 30 0C/min -; 180 0C ^ 4 0C/min -; 270 0C (15 min); CAS no: 90982; Active phase: Ultra-2; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Hernandez, F.; Morell, I.; Beltran, J.; Lopez, F. J., Multi-residue procedure for the analysis of pesticides in groundwater: Application to samples from the Comunidad Valenciana, Spain, Chromatographia, 37(5/6), 1993, 303-312.)NIST Spectranist ri  |
| 1955. 3 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column type: Capillary; Description: 110 0C (1 min) ^ 15 0C/min -; 190 0C ^ 3 0C/min -; 270 0C (50 min); CAS no: 90982; Active phase: DB-5; Data type: Normal alkane RI; Authors: Hopper, M. L., Analysis of organochlorine presticide residues using simultaneous injection of two capillary columns with electron capture and electrolytic conductivity detectors, J. Ass. Offic. Anal. Chem, 74(6), 1991, 974-981.)NIST Spectranist ri  |

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

|  |  |
| --- | --- |
| Density:  | 1. 3±0. 1 g/cm 3  |
| Boiling Point:  | 353. 0±0. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 7 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 59. 8±3. 0 kJ/mol  |
| Flash Point:  | 156. 2±24. 3 °C  |
| Index of Refraction:  | 1. 604  |
| Molar Refractivity:  | 65. 8±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 2  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 4. 62  |
| ACD/LogD (pH 5. 5):  | 4. 69  |
| ACD/BCF (pH 5. 5):  | 2168. 54  |
| ACD/KOC (pH 5. 5):  | 8504. 05  |
| ACD/LogD (pH 7. 4):  | 4. 69  |
| ACD/BCF (pH 7. 4):  | 2168. 54  |
| ACD/KOC (pH 7. 4):  | 8504. 05  |
| Polar Surface Area:  | 17 Å 2  |
| Polarizability:  | 26. 1±0. 5 10 -24 cm 3  |
| Surface Tension:  | 46. 0±3. 0 dyne/cm  |
| Molar Volume:  | 191. 4±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) = 4. 44Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 342. 22 (Adapted Stein & Brown method)Melting Pt (deg C): 107. 69 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 6. 39E-006 (Modified Grain method)MP (exp database): 147. 5 deg CBP (exp database): 353 deg CSubcooled liquid VP: 0. 000112 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 3. 796log Kow used: 4. 44 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 7. 802 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 07E-006 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 5. 562E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 44 (KowWin est)Log Kaw used: -4. 359 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 8. 799Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2700Biowin2 (Non-Linear Model) : 0. 0064Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 2086 (months )Biowin4 (Primary Survey Model) : 3. 1325 (weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 1609Biowin6 (MITI Non-Linear Model): 0. 0333Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -1. 1238Ready 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. 0149 Pa (0. 000112 mm Hg)Log Koa (Koawin est ): 8. 799Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 000201 Octanol/air (Koa) model: 0. 000155 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0072 Mackay model : 0. 0158 Octanol/air (Koa) model: 0. 0122 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 2. 5007 E-12 cm3/molecule-secHalf-Life = 4. 277 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 51. 325 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 0115 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 2826Log Koc: 3. 451 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 = 1. 876 (BCF = 75. 13)log Kow used: 4. 44 (estimated)Volatilization from Water: Henry LC: 1. 07E-006 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 868. 7 hours (36. 2 days)Half-Life from Model Lake : 9610 hours (400. 4 days)Removal In Wastewater Treatment: Total removal: 52. 85 percentTotal biodegradation: 0. 50 percentTotal sludge adsorption: 52. 33 percentTotal to Air: 0. 03 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 827 103 1000 Water 11. 2 1. 44e+003 1000 Soil 78. 4 2. 88e+003 1000 Sediment 9. 59 1. 3e+004 0 Persistence Time: 2e+003 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop