

4,4'-

dichlorobenzophenon  
e  $C_{13}H_8Cl_2O$  structure



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## Contents

- Retention Index (Normal Alkane):

Molecular

$C_{13}H_8Cl_2O$

Formula

Average mass 251. 108 Da

Density 1. 3±0. 1 g/cm<sup>3</sup>

Boiling Point 353. 0±0. 0 °C at  
760 mmHg

Flash Point 156. 2±24. 3 °C

Molar	
Refractivity	65. 8±0. 3 cm <sup>3</sup>
Polarizability	26. 1±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface	
Tension	46. 0±3. 0 dyne/cm
Molar Volume	191. 4±3. 0 cm <sup>3</sup>

- 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

°CLabNetworkLN00206

828

144-146 °CIndofine[CS-

280]

- **Experimental Boiling Point:**

352-354 °CAlfa

AesarA12608

353 °CSynQuest2617-

5-05

353 °CBiosynthW-

100319

353

°CLabNetworkLN00206

828

- **Experimental LogP:**

4. 623Vitas-

MSTK290986

- **Experimental Flash Point:**

156 °CBiosynthW-

100319

352-354

°CLabNetworkLN00206

828

- **Experimental Gravity:**

156 g/mL BiosynthW-

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 °C(1  
min) ^ 25 °C/min -;  
125 °C ^ 10 °C/min -;  
300 °C (10 min); CAS  
no: 90982; Active  
phase: 5 % Phenyl  
methyl siloxane;  
Carrier gas: Helium;  
Phase thickness: 0.25  
µm; 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

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 °C(1

min) ^ 25 °C/min -;

125 °C ^ 10 °C/min -;

300 °C (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 additives, 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  $\mu\text{m}$ ;  
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

pesticide 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 <sup>3</sup>
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 <sup>3</sup>
#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 <sup>2</sup>
Polarizability:	26. 1±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	46. 0±3. 0 dyne/cm
Molar Volume:	191. 4±3. 0 cm <sup>3</sup>

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

<https://assignbuster.com/44-dichlorobenzophenone-c13h8cl2o-structure/>

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