

# [2,4,6-trichloroanisole c7h5cl3o structure](https://assignbuster.com/246-trichloroanisole-c7h5cl3o-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 7 H 5 Cl 3 O  |
| Average mass  | 211. 473 Da  |
| Density  | 1. 4±0. 1 g/cm 3  |
| Boiling Point  | 246. 0±0. 0 °C at 760 mmHg  |
| Flash Point  | 100. 4±26. 0 °C  |
| Molar Refractivity  | 47. 6±0. 3 cm 3  |
| Polarizability  | 18. 9±0. 5 10 -24 cm 3  |
| Surface Tension  | 38. 4±3. 0 dyne/cm  |
| Molar Volume  | 149. 3±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 60 °CTCIT0867  |
| 60-62 °COxford University Chemical Safety Data (No longer updated)More details  |
| 61 °CJean-Claude Bradley Open Melting Point Dataset14933  |
| 61. 5 °CJean-Claude Bradley Open Melting Point Dataset21028  |
| 61-62 °CFooDBFDB000814  |

## Experimental Boiling Point:

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| 132 °COxford University Chemical Safety Data (No longer updated)More details  |
| 738 °C / 240 mmHg (840. 0944 °C / 760 mmHg)FooDBFDB000814  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

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| --- |
| 60 °CTCI  |
| 60 °CTCIT0867  |

* Miscellaneous

## Appearance:

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| --- |
| white or off-white fibrous powderOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

|  |
| --- |
| Stable. Incompatible with strong oxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

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| Safety glasses, adequate ventilation. Oxford University Chemical Safety Data (No longer updated)More details  |

* Gas Chromatography

## Retention Index (Kovats):

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| 1409 (estimated with error: 89)NIST Spectramainlib\_333450, replib\_69785, replib\_100136, replib\_238004, replib\_249011  |
| 1339 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 25 mm; Column type: Capillary; CAS no: 87401; Active phase: Methyl Silicone; Data type: Kovats RI; Authors: Staples, E. J., Ultrahigh-speed chromatography and virtual chemical sensors for detecting explosives and chemical warfare agents, IEEE Sens. J., 5(4), 2005, 622-631.)NIST Spectranist ri  |
| 1319 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 3 mm; Column length: 25 m; Column type: Capillary; Start T: 140 C; CAS no: 87401; Active phase: SE-30; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1333 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 3 mm; Column length: 25 m; Column type: Capillary; Start T: 160 C; CAS no: 87401; Active phase: SE-30; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1350 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 3 mm; Column length: 25 m; Column type: Capillary; Start T: 180 C; CAS no: 87401; Active phase: SE-30; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1813 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Start T: 140 C; CAS no: 87401; Active phase: OV-351; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1837 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Start T: 160 C; CAS no: 87401; Active phase: OV-351; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1842 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Start T: 180 C; CAS no: 87401; Active phase: OV-351; Carrier gas: N2; Data type: Kovats RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

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| 1322 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 55 m; Column type: Capillary; Description: 40C(3min) => 20C/min => 80C => 2C/min=> 240C(45min); CAS no: 87401; Active phase: CP Sil 2; Carrier gas: N2; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Fuhrer, U.; Deissler, A.; Schreitmuller, J.; Ballschmiter, K., Analysis of Halogenated Methoxybenzenes and Hexachlorobenzene (HCB) in the Picogram m-3 Range in Marine Air, Chromatographia, 45, 1997, 414-427.)NIST Spectranist ri  |
| 1298 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 80 C; End T: 260 C; CAS no: 87401; Active phase: Ultra-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Okumura, T., retention indices of environmental chemicals on methyl silicone capillary column, Journal of Environmental Chemistry (Japan), 1(2), 1991, 333-358.)NIST Spectranist ri  |
| 1307. 9 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 1. 8 m; Column type: Packed; CAS no: 87401; Active phase: OV-101; Carrier gas: N2; Substrate: Chromosorb W HP; Data type: Normal alkane RI; Authors: Yurawecz, M. P.; Puma, B. J., Gas chromatographic determination of electron capture sensitive volatile industrial chemical residues in foods, using AOAC pesticide multiresidue extraction and cleanup procedures, J. Ass. Offic. Anal. Chem, 69(1), 1986, 80-86.)NIST Spectranist ri  |
| 1330 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40 0C ^ 2 0C/min -> 12 0C/min -> 105 0C ^ 6 0C/min -> 220 0C (20 min); CAS no: 87401; Active phase: DB-5; Carrier gas: Hydrogen; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Prat, C.; Trias, R.; Cullere, L.; Escudero, A.; Antico, E.; BAneras, L., Off-odor compounds produced in cork by isolated bacteria and fungi: a gas chromatography – mass spectrometry and gas chromatography – olfactometry study, J. Agric. Food Chem., 57(16), 2009, 7473-7479.)NIST Spectranist ri  |
| 1291 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 3 mm; Column length: 30 m; Column type: Capillary; Heat rate: 16 K/min; Start T: 80 C; End T: 250 C; CAS no: 87401; Active phase: DB-5; Carrier gas: H2; Data type: Normal alkane RI; Authors: Spadone, J.-C.; Takeoka, G.; Liardon, R., Analytical Investigation of Rio Off-Flavor in Green Coffee, J. Agric. Food Chem., 38(1), 1990, 226-233.)NIST Spectranist ri  |
| 1345 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 3 mm; Column length: 50 m; Column type: Capillary; Heat rate: 16 K/min; Start T: 80 C; End T: 250 C; CAS no: 87401; Active phase: HP-5; Carrier gas: H2; Data type: Normal alkane RI; Authors: Spadone, J.-C.; Takeoka, G.; Liardon, R., Analytical Investigation of Rio Off-Flavor in Green Coffee, J. Agric. Food Chem., 38(1), 1990, 226-233.)NIST Spectranist ri  |
| 1806 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40 0C (5 min) ^ 4 0C/min -> 100 0C ^ 6 0C/min -> 220 0C (40 min); CAS no: 87401; Active phase: DB-Wax; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Ferreira, V.; Juan, F. S.; Escudero, A.; Cullere, L.; Fernandez-Zurbano, P.; Saenz-Navajas, M. P.; Cacho, J., Modeling quality of premium Spanish red wines from gas chromatography-olfactometry data, J. Agr. Food. Chem., 57(16), 2009, 7490-7498.)NIST Spectranist ri  |
| 1832 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Description: 40 0C ^ 2 0C/min -> 12 0C/min -> 105 0C ^ 6 0C/min -> 220 0C (20 min); CAS no: 87401; Active phase: DB-Wax; Carrier gas: Hydrogen; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Prat, C.; Trias, R.; Cullere, L.; Escudero, A.; Antico, E.; BAneras, L., Off-odor compounds produced in cork by isolated bacteria and fungi: a gas chromatography – mass spectrometry and gas chromatography – olfactometry study, J. Agric. Food Chem., 57(16), 2009, 7473-7479.)NIST Spectranist ri  |
| 1812 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 25C(8min) => 4C/min => 60C => 6C/min => 160C => 20C/min => 200C; CAS no: 87401; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Caldentey, P.; Daria Fumi, M.; Mazzoleni, V.; Careri, M., Volatile compounds produced by microorganisms isolated from cork, Flavour Fragr. J., 13, 1998, 185-188.)NIST Spectranist ri  |

## Retention Index (Linear):

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| 1331 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; CAS no: 87401; Active phase: PONA; Data type: Linear RI; Authors: Cantergiani, E.; Brevard, H.; Krebs, Y.; Feria-Morales, A.; Amado, R.; Yeretzian, C., Characterisation of the aroma of green Mexican coffee and identification of mouldy/earthy defect, Eur. Food Res. Technol., 212, 2001, 648-657.)NIST Spectranist ri  |
| 1305 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 3 mm; Column length: 25 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 100 C; CAS no: 87401; Active phase: SE-30; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1319 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 3 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; CAS no: 87401; Active phase: SE-30; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1327 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 3 mm; Column length: 25 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 100 C; CAS no: 87401; Active phase: SE-30; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1350. 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: Multi-step temperature program; T(initial)= 60C; T(final)= 270C; CAS no: 87401; Active phase: VF-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Tret’yakov, K. V., Retention Data. NIST Mass Spectrometry Data Center., 2007.)NIST Spectranist ri  |
| 1817 (Program type: Complex; Column… (show more)class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 20C(30s) =; fast=; 60C =; 4C/min =; 220C (20min); CAS no: 87401; Active phase: DB-Wax; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Cantergiani, E.; Brevard, H.; Krebs, Y.; Feria-Morales, A.; Amado, R.; Yeretzian, C., Characterisation of the aroma of green Mexican coffee and identification of mouldy/earthy defect, Eur. Food Res. Technol., 212, 2001, 648-657.)NIST Spectranist ri  |
| 1775 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 100 C; CAS no: 87401; Active phase: OV-351; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1794 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 100 C; CAS no: 87401; Active phase: OV-351; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |
| 1805 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 100 C; CAS no: 87401; Active phase: OV-351; Carrier gas: N2; Data type: Linear RI; Authors: Korhonen, I. O. O., Gas-Liquid Chromatographic Analyses. XXVIII. Capillary Column Studies of Chlorinated Anisoles, J. Chromatogr., 294, 1984, 99-116.)NIST Spectranist ri  |

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

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| --- | --- |
| Density:  | 1. 4±0. 1 g/cm 3  |
| Boiling Point:  | 246. 0±0. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 4 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 46. 4±3. 0 kJ/mol  |
| Flash Point:  | 100. 4±26. 0 °C  |
| Index of Refraction:  | 1. 551  |
| Molar Refractivity:  | 47. 6±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 1  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 3. 95  |
| ACD/LogD (pH 5. 5):  | 3. 87  |
| ACD/BCF (pH 5. 5):  | 516. 59  |
| ACD/KOC (pH 5. 5):  | 3045. 60  |
| ACD/LogD (pH 7. 4):  | 3. 87  |
| ACD/BCF (pH 7. 4):  | 516. 59  |
| ACD/KOC (pH 7. 4):  | 3045. 60  |
| Polar Surface Area:  | 9 Å 2  |
| Polarizability:  | 18. 9±0. 5 10 -24 cm 3  |
| Surface Tension:  | 38. 4±3. 0 dyne/cm  |
| Molar Volume:  | 149. 3±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. 01Log Kow (Exper. database match) = 4. 11Exper. Ref: Opperhuizen, A & Voors, PI (1987)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 245. 41 (Adapted Stein & Brown method)Melting Pt (deg C): 43. 58 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0193 (Modified Grain method)MP (exp database): 61. 5 deg CBP (exp database): 241 deg CSubcooled liquid VP: 0. 0422 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): 11. 8log Kow used: 4. 11 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 10 mg/L (20 deg C)Exper. Ref: PIRBAZARI, M ET AL (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 14. 329 mg/LWat Sol (Exper. database match) = 10. 00Exper. Ref: PIRBAZARI, M ET AL (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 30E-004 atm-m3/moleGroup Method: 2. 68E-003 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 551E-004 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 11 (exp database)Log Kaw used: -2. 275 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 6. 385Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 2315Biowin2 (Non-Linear Model) : 0. 0220Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 0539 (months )Biowin4 (Primary Survey Model) : 3. 1237 (weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3136Biowin6 (MITI Non-Linear Model): 0. 0657Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 4631Ready 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): 5. 63 Pa (0. 0422 mm Hg)Log Koa (Koawin est ): 6. 385Kp (particle/gas partition coef. (m3/ug)): Mackay model : 5. 33E-007 Octanol/air (Koa) model: 5. 96E-007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 93E-005 Mackay model : 4. 27E-005 Octanol/air (Koa) model: 4. 77E-005 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 1. 4167 E-12 cm3/molecule-secHalf-Life = 7. 550 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 90. 597 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 3. 1E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 521. 4Log Koc: 2. 717 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 = 2. 465 (BCF = 291. 5)log Kow used: 4. 11 (expkow database)Volatilization from Water: Henry LC: 0. 00268 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 802 hoursHalf-Life from Model Lake : 141. 6 hours (5. 9 days)Removal In Wastewater Treatment: Total removal: 64. 61 percentTotal biodegradation: 0. 23 percentTotal sludge adsorption: 28. 28 percentTotal to Air: 36. 10 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 3. 79 181 1000 Water 7. 53 1. 44e+003 1000 Soil 85. 7 2. 88e+003 1000 Sediment 2. 95 1. 3e+004 0 Persistence Time: 1. 18e+003 hr

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* 1-Click Scaffold Hop