

# [Dicyclohexyl phthalate c20h26o4 structure](https://assignbuster.com/dicyclohexyl-phthalate-c20h26o4-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula | C 20 H 26 O 4 |
| Average mass | 330. 418 Da |
| Density | 1. 1±0. 1 g/cm 3 |
| Boiling Point | 425. 8±18. 0 °C at 760 mmHg |
| Flash Point | 206. 6±19. 6 °C |
| Molar Refractivity | 91. 2±0. 4 cm 3 |
| Polarizability | 36. 1±0. 5 10 -24 cm 3 |
| Surface Tension | 45. 8±5. 0 dyne/cm |
| Molar Volume | 288. 6±5. 0 cm 3 |

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

## Experimental Melting Point:

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| --- |
| 65 °CTCIP0293 |
| 62-64 °CMerck Millipore1191, 800920 |
| 66 °CJean-Claude Bradley Open Melting Point Dataset21072 |
| 63-67 °CAlfa AesarH56004 |
| 63-67 °C (Literature)LabNetworkLN00223414 |

## Experimental Boiling Point:

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| --- |
| 200-235 °C / 4 mmHg (426. 6939-476. 9317 °C / 760 mmHg)LabNetworkLN00223414 |

## Experimental Flash Point:

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| --- |
| 207 °CLabNetworkLN00223414 |

## Experimental Gravity:

|  |
| --- |
| 1. 383 g/mLAlfa AesarH56004 |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 65 °CTCI |
| 65 °CTCIP0293 |

* Miscellaneous

## Safety:

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| --- |
| 26-37-60Alfa AesarH56004 |
| 36/37/38Alfa AesarH56004 |
| GHS07BiosynthW-104111 |
| H315; H319; H335BiosynthW-104111 |
| H315-H319-H335Alfa AesarH56004 |
| IrritantSynQuest2623-1-58 |
| P261; P305+P351+P338BiosynthW-104111 |
| P261-P280-P305+P351+P338-P304+P340-P405-P501aAlfa AesarH56004 |
| WarningAlfa AesarH56004 |
| WarningBiosynthW-104111 |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 2561 (estimated with error: 47)NIST Spectramainlib\_250710, replib\_232967, replib\_313012, replib\_315339 |
| 2453 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 1. 5 m; Column type: Packed; CAS no: 84617; Active phase: SE-30; Carrier gas: He; Substrate: Chromosorb G HP (80-100 mesh); Data type: Kovats RI; Authors: Ramsey, J. D.; Lee, T. D.; Osselton, M. D.; Moffat, A. C., Gas-liquid chromatographic retention indices of 296 non-drug substances on SE-30 or OV-1 likely to be encountered in toxicological analyses, J. Chromatogr., 184, 1980, 185-206.)NIST Spectranist ri |
| 2461 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column length: 1. 5 m; Column type: Packed; CAS no: 84617; Active phase: SE-30; Carrier gas: He; Substrate: Chromosorb G HP (80-100 mesh); Data type: Kovats RI; Authors: Ramsey, J. D.; Lee, T. D.; Osselton, M. D.; Moffat, A. C., Gas-liquid chromatographic retention indices of 296 non-drug substances on SE-30 or OV-1 likely to be encountered in toxicological analyses, J. Chromatogr., 184, 1980, 185-206.)NIST Spectranist ri |
| 2475 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 3 mm; Column length: 50 m; Column type: Capillary; Start T: 250 C; CAS no: 84617; Active phase: SE-30; Carrier gas: He; Phase thickness: 0. 39 um; Data type: Kovats RI; Authors: Friocourt, M. P.; Berthou, F.; Picart, D.; Dreano, Y.; Floch, H. H., Glass Capillary Column Gas Chromatography of Phthalate Esters, J. Chromatogr., 172, 1979, 261-271.)NIST Spectranist ri |

## Retention Index (Normal Alkane):

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| --- |
| 2434 (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: 84617; 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 |
| 2454. 2 (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: 84617; 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 |
| 2453 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Other; CAS no: 84617; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.)NIST Spectranist ri |
| 2461 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Other; CAS no: 84617; Active phase: Methyl Silicone; Data type: Normal alkane RI; Authors: Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.)NIST Spectranist ri |
| 2483. 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: 80C(1min) => 50C/min => 200C => 15C/min => 350C (2min); CAS no: 84617; Active phase: DB-5MS; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: George, C.; Prest, H., A new approach to the analysis of phthalate esters by GC/MS, 2003.)NIST Spectranist ri |
| 2511. 3 (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: 84617; 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 |
| 2468 (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: 15 K/min; Start T: 120 C; End T: 160 C; End time: 16 min; CAS no: 84617; Active phase: DB-5; Data type: Normal alkane RI; Authors: Lopez-Avila, V.; Milanes, J.; Beckert, W. F., Single-laboratory evaluation of method 8060 for the determination of phthalates in environmental samples, J. Ass. Offic. Anal. Chem, 74(5), 1991, 793-808.)NIST Spectranist ri |
| 2516. 1 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 53 mm; Column length: 30 m; Column type: Capillary; Description: 150 0C (0. 5 min) ^ 3 0C/min -> 220 0C ^ 5 0C/min -> 275 0C (15 min); CAS no: 84617; Active phase: DB-5; Data type: Normal alkane RI; Authors: Lopez-Avila, V.; Milanes, J.; Beckert, W. F., Single-laboratory evaluation of method 8060 for the determination of phthalates in environmental samples, J. Ass. Offic. Anal. Chem, 74(5), 1991, 793-808.)NIST Spectranist ri |

## Retention Index (Linear):

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| 2472 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Packed; Heat rate: 10 K/min; Start T: 100 C; End T: 340 C; CAS no: 84617; Active phase: SE-30; Carrier gas: N2; Substrate: Chromosorb Q; Data type: Linear RI; Authors: Messadi, D.; Vergnaud, J.-M., Quick identification and analysis of plasticizers in PVC by programmed-temperature gas chromatography using the best stationary phases, J. Appl. Polym. Sci., 24, 1979, 1215-1225.)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: | 425. 8±18. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±1. 0 mmHg at 25°C |
| Enthalpy of Vaporization: | 68. 0±3. 0 kJ/mol |
| Flash Point: | 206. 6±19. 6 °C |
| Index of Refraction: | 1. 544 |
| Molar Refractivity: | 91. 2±0. 4 cm 3 |
| #H bond acceptors: | 4 |
| #H bond donors: | 0 |
| #Freely Rotating Bonds: | 6 |
| #Rule of 5 Violations: | 1 |

|  |  |
| --- | --- |
| ACD/LogP: | 5. 76 |
| ACD/LogD (pH 5. 5): | 5. 32 |
| ACD/BCF (pH 5. 5): | 6482. 34 |
| ACD/KOC (pH 5. 5): | 18622. 12 |
| ACD/LogD (pH 7. 4): | 5. 32 |
| ACD/BCF (pH 7. 4): | 6482. 34 |
| ACD/KOC (pH 7. 4): | 18622. 12 |
| Polar Surface Area: | 53 Å 2 |
| Polarizability: | 36. 1±0. 5 10 -24 cm 3 |
| Surface Tension: | 45. 8±5. 0 dyne/cm |
| Molar Volume: | 288. 6±5. 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) = 6. 20Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 394. 85 (Adapted Stein & Brown method)Melting Pt (deg C): 61. 45 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 4. 58E-006 (Modified Grain method)MP (exp database): 66 deg CBP (exp database): 218 @ 4. 5 mm Hg deg CVP (exp database): 8. 69E-07 mm Hg at 25 deg CSubcooled liquid VP: 2. 21E-006 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): 0. 04098log Kow used: 6. 20 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 4 mg/L (24 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 2. 4027 mg/LWat Sol (Exper. database match) = 4. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 39E-007 atm-m3/moleGroup Method: 6. 43E-008 atm-m3/moleExper Database: 1. 00E-07 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 859E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 6. 20 (KowWin est)Log Kaw used: -5. 388 (exp database)Log Koa (KOAWIN v1. 10 estimate): 11. 588Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 9386Biowin2 (Non-Linear Model) : 0. 9985Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7494 (weeks-months)Biowin4 (Primary Survey Model) : 3. 8289 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6716Biowin6 (MITI Non-Linear Model): 0. 6144Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 3232Ready 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. 000295 Pa (2. 21E-006 mm Hg)Log Koa (Koawin est ): 11. 588Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 0102 Octanol/air (Koa) model: 0. 0951 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 269 Mackay model : 0. 449 Octanol/air (Koa) model: 0. 884 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 24. 2718 E-12 cm3/molecule-secHalf-Life = 0. 441 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 5. 288 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 359 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 764E+004Log Koc: 4. 246 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 1. 883E-002 L/mol-secKb Half-Life at pH 8: 1. 166 years Kb Half-Life at pH 7: 11. 662 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 4. 076 (BCF = 1. 191e+004)log Kow used: 6. 20 (estimated)Volatilization from Water: Henry LC: 1E-007 atm-m3/mole (Henry experimental database)Half-Life from Model River: 1. 064E+004 hours (443. 5 days)Half-Life from Model Lake : 1. 163E+005 hours (4845 days)Removal In Wastewater Treatment: Total removal: 92. 84 percentTotal biodegradation: 0. 77 percentTotal sludge adsorption: 92. 07 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 113 10. 6 1000 Water 3. 16 900 1000 Soil 37 1. 8e+003 1000 Sediment 59. 7 8. 1e+003 0 Persistence Time: 2. 88e+003 hr

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* 1-Click Scaffold Hop