

# [Methylcyclopentadiene c6h8 structure](https://assignbuster.com/methylcyclopentadiene-c6h8-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 6 H 8  |
| Average mass  | 80. 128 Da  |
| Density  | 0. 9±0. 1 g/cm 3  |
| Boiling Point  | 85. 8±7. 0 °C at 760 mmHg  |
| Flash Point  | -15. 3±13. 0 °C  |
| Molar Refractivity  | 27. 0±0. 3 cm 3  |
| Polarizability  | 10. 7±0. 5 10 -24 cm 3  |
| Surface Tension  | 26. 8±3. 0 dyne/cm  |
| Molar Volume  | 93. 3±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Gas Chromatography

## Retention Index (Kovats):

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| --- |
| 653 (estimated with error: 39)NIST Spectramainlib\_164279  |
| 642 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 23 mm; Column length: 25 m; Column type: Capillary; Start T: 80 C; CAS no: 96399; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Bermejo, J.; Blanco, C. G.; Diez, M. A.; Guillen, M. D., Kovats retention indices of selected mono and polycyclic olefins, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 10, 1987, 461-463., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 23 mm; Column length: 25 m; Column type: Capillary; Start T: 80 C; CAS no: 96399; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; Bermejo, J., Chromatographic study of methylcyclopentadiene dimers and iso-dimers and determination of their boiling points, J. Chromatogr., 508, 1990, 363-374.)NIST Spectranist ri  |
| 644 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 12 m; Column type: Capillary; Start T: 100 C; CAS no: 96399; Active phase: BP-1; Carrier gas: N2; Data type: Kovats RI; Authors: Bermejo, J.; Blanco, C. G.; Diez, M. A.; Guillen, M. D., Kovats retention indices of selected mono and polycyclic olefins, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 10, 1987, 461-463., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 23 mm; Column length: 25 m; Column type: Capillary; Start T: 100 C; CAS no: 96399; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Bermejo, J.; Blanco, C. G.; Diez, M. A.; Guillen, M. D., Kovats retention indices of selected mono and polycyclic olefins, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 10, 1987, 461-463., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 23 mm; Column length: 25 m; Column type: Capillary; Start T: 100 C; CAS no: 96399; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; Bermejo, J., Chromatographic study of methylcyclopentadiene dimers and iso-dimers and determination of their boiling points, J. Chromatogr., 508, 1990, 363-374.)NIST Spectranist ri  |
| 641 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 12 m; Column type: Capillary; Start T: 80 C; CAS no: 96399; Active phase: BP-1; Carrier gas: N2; Data type: Kovats RI; Authors: Bermejo, J.; Blanco, C. G.; Diez, M. A.; Guillen, M. D., Kovats retention indices of selected mono and polycyclic olefins, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 10, 1987, 461-463.)NIST Spectranist ri  |
| 627. 5 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 5 mm; Column length: 45 m; Column type: Capillary; Start T: 80 C; CAS no: 96399; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; Bermejo, J., Chromatographic study of methylcyclopentadiene dimers and iso-dimers and determination of their boiling points, J. Chromatogr., 508, 1990, 363-374.)NIST Spectranist ri  |
| 630 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 5 mm; Column length: 45 m; Column type: Capillary; Start T: 100 C; CAS no: 96399; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; Bermejo, J., Chromatographic study of methylcyclopentadiene dimers and iso-dimers and determination of their boiling points, J. Chromatogr., 508, 1990, 363-374.)NIST Spectranist ri  |
| 652. 8 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 80 C; CAS no: 96399; Active phase: SE-54; Carrier gas: N2; Data type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; Bermejo, J., Chromatographic study of methylcyclopentadiene dimers and iso-dimers and determination of their boiling points, J. Chromatogr., 508, 1990, 363-374.)NIST Spectranist ri  |
| 653. 8 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Start T: 100 C; CAS no: 96399; Active phase: SE-54; Carrier gas: N2; Data type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; Bermejo, J., Chromatographic study of methylcyclopentadiene dimers and iso-dimers and determination of their boiling points, J. Chromatogr., 508, 1990, 363-374.)NIST Spectranist ri  |
| 626 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 49 C; CAS no: 96399; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 64 C; CAS no: 96399; Active phase: Squalane; Carrier gas: H2; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Sojak, L.; Ruman, J.; Janak, J., Characterization of Monoalkylcyclopentadiens by Retention-Structure Correlation in Capillary Gas Chromatography, J. Chromatogr., 391, 1987, 79-87.)NIST Spectranist ri  |
| 626. 3 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Start T: 50 C; CAS no: 96399; Active phase: Squalane; Data type: Kovats RI; Authors: Bajus, M.; Vesely, V.; Leclercq, P. A.; Rijks, J. A., Steam cracking of hydrocarbons. 2. Pyrolysis of methylcyclohexane, Ind. Eng. Chem. Prod. Res. Dev., 18(2), 1979, 135-142.)NIST Spectranist ri  |
| 623 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 27 C; CAS no: 96399; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri  |
| 628 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: Packed; Start T: 67 C; CAS no: 96399; Active phase: Squalane; Carrier gas: He; Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Gas Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri  |
| 844. 5 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capillary; Start T: 64 C; CAS no: 96399; Active phase: Carbowax 20M; Carrier gas: H2; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Sojak, L.; Ruman, J.; Janak, J., Characterization of Monoalkylcyclopentadiens by Retention-Structure Correlation in Capillary Gas Chromatography, J. Chromatogr., 391, 1987, 79-87.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

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| --- |
| 659. 3 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 1 mm; Column length: 20 m; Column type: Capillary; Description: 40C(0. 4min) => 10C/min=> 110C=> 20C/min => 260C (1min); CAS no: 96399; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 4 um; Data type: Normal alkane RI; Authors: LECO Corporation, Rapid qualitative GC/TOFMS analysis of unleaded gasoline, 2003.)NIST Spectranist ri  |
| 638. 8 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 1 mm; Column length: 20 m; Column type: Capillary; Description: 40C(0. 4min) => 10C/min => 110C => 20C/min => 260C (1min); CAS no: 96399; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 4 um; Data type: Normal alkane RI; Authors: LECO Corporation, Rapid qualitative GC/TOFMS analysis of a petroleum refinery reformate standard, 2003.)NIST Spectranist ri  |
| 626 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 96399; Active phase: Squalane; Data type: Normal alkane RI; Authors: Chen, H.-F., Quantitative prediction of gas chromatography retention indices with support vector machines, radial basis neutral networks and multiple linear regression, Anal. Chim. Acta, 609, 2008, 24-36.)NIST Spectranist ri  |

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

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| --- | --- |
| Density:  | 0. 9±0. 1 g/cm 3  |
| Boiling Point:  | 85. 8±7. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 76. 5±0. 1 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 31. 3±0. 8 kJ/mol  |
| Flash Point:  | -15. 3±13. 0 °C  |
| Index of Refraction:  | 1. 490  |
| Molar Refractivity:  | 27. 0±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 2. 38  |
| ACD/LogD (pH 5. 5):  | 2. 85  |
| ACD/BCF (pH 5. 5):  | 86. 09  |
| ACD/KOC (pH 5. 5):  | 844. 60  |
| ACD/LogD (pH 7. 4):  | 2. 85  |
| ACD/BCF (pH 7. 4):  | 86. 09  |
| ACD/KOC (pH 7. 4):  | 844. 60  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 10. 7±0. 5 10 -24 cm 3  |
| Surface Tension:  | 26. 8±3. 0 dyne/cm  |
| Molar Volume:  | 93. 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) = 2. 80Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 91. 79 (Adapted Stein & Brown method)Melting Pt (deg C): -73. 33 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 128 (Mean VP of Antoine & Grain methods)BP (exp database): 72. 78 deg CVP (exp database): 1. 24E+02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 153. 7log Kow used: 2. 80 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1102. 8 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 9. 96E-002 atm-m3/moleGroup Method: 1. 17E-002 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 8. 780E-002 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 80 (KowWin est)Log Kaw used: 0. 610 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 190Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7094Biowin2 (Non-Linear Model) : 0. 8666Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0221 (weeks )Biowin4 (Primary Survey Model) : 3. 7321 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5125Biowin6 (MITI Non-Linear Model): 0. 6350Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 4159Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 0. 4617BioHC Half-Life (days) : 2. 8956Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 1. 65E+004 Pa (124 mm Hg)Log Koa (Koawin est ): 2. 190Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 81E-010 Octanol/air (Koa) model: 3. 8E-011 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 6. 55E-009 Mackay model : 1. 45E-008 Octanol/air (Koa) model: 3. 04E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 190. 7338 E-12 cm3/molecule-secHalf-Life = 0. 056 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 673 HrsOzone Reaction: OVERALL Ozone Rate Constant = 100. 000000 E-17 cm3/molecule-secHalf-Life = 0. 011 Days (at 7E11 mol/cm3)Half-Life = 16. 502 MinReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 1. 05E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 145. 3Log Koc: 2. 162 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. 457 (BCF = 28. 67)log Kow used: 2. 80 (estimated)Volatilization from Water: Henry LC: 0. 0117 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 0. 9582 hours (57. 49 min)Half-Life from Model Lake : 85. 51 hours (3. 563 days)Removal In Wastewater Treatment: Total removal: 82. 31 percentTotal biodegradation: 0. 04 percentTotal sludge adsorption: 2. 16 percentTotal to Air: 80. 11 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 246 0. 228 1000 Water 60 360 1000 Soil 39 720 1000 Sediment 0. 696 3. 24e+003 0 Persistence Time: 104 hr

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