

Methylcyclopentadien e C_6H_8 structure



Contents

- Retention Index (Normal Alkane):

Molecular Formula	C_6H_8
Average mass	80. 128 Da
Density	$0.9 \pm 0.1 \text{ g/cm}^3$
Boiling Point	$85.8 \pm 7.0 \text{ }^\circ\text{C}$ at 760 mmHg
Flash Point	$-15.3 \pm 13.0 \text{ }^\circ\text{C}$
Molar Refractivity	$27.0 \pm 0.3 \text{ cm}^3$
Polarizability	$10.7 \pm 0.5 \cdot 10^{-24} \text{ cm}^3$
Surface Tension	$26.8 \pm 3.0 \text{ dyne/cm}$
Molar Volume	$93.3 \pm 3.0 \text{ cm}^3$

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

- **Retention Index (Kovats):**

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. 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 RI 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

type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; Bermejo
Chromatographic study of methylcyclopentadiene dimers and iso-dimers
determination of their boiling points, J. Chromatogr., 508, 1990, 363-374
Spectranist ri

652. 8 (Program type: Isothermal; Col... (show more)umn class: Semi-sta
non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column ty
Capillary; Start T: 80 C; CAS no: 96399; Active phase: SE-54; Carrier gas:
Data type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; B
J., Chromatographic study of methylcyclopentadiene dimers and iso-dime
determination of their boiling points, J. Chromatogr., 508, 1990, 363-374
Spectranist ri

653. 8 (Program type: Isothermal; Col... (show more)umn class: Semi-sta
non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column ty
Capillary; Start T: 100 C; CAS no: 96399; Active phase: SE-54; Carrier gas:
Data type: Kovats RI; Authors: Diez, M. A.; Guillen, M. D.; Blanco, C. G.; B
J., Chromatographic study of methylcyclopentadiene dimers and iso-dime
determination of their boiling points, J. Chromatogr., 508, 1990, 363-374
Spectranist ri

626 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column diameter: 0. 25 mm; Column length: 50 ft; Column type: P
Start T: 49 C; CAS no: 96399; Active phase: Squalane; Carrier gas: He; Su
Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E.,
Variation of the retention index with temperature on squalane substrates
Chromatogr., 6, 1968, 203-217., Program type: Isothermal; Col... (show

more)umn class: Semi-standard non-polar; Column diameter: 0.25 mm; length: 50 m; Column type: Capillary; Start T: 64 C; CAS no: 96399; Active phase: Squalane; Carrier gas: H₂; Phase thickness: 0.25 μm; Data type: Kovats RI; Authors: Sojak, L.; Ruman, J.; Janak, J., Characterization of Monoalkylcyclopentadienes by Retention-Structure Correlation in Capillary 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: Porapak Q; Start T: 27 C; CAS no: 96399; Active phase: Squalane; Carrier gas: He; Stationary phase: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. 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: Porapak Q; Start T: 67 C; CAS no: 96399; Active phase: Squalane; Carrier gas: He; Stationary phase: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hinton, R. E., Variation of the retention index with temperature on squalane substrates, J. Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri

Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri

844. 5 (Program type: Isothermal; Col... (show more)umn class: Standard

Column diameter: 0. 25 mm; Column length: 50 m; Column type: Capilla

T: 64 C; CAS no: 96399; Active phase: Carbowax 20M; Carrier gas: H2; PH

thickness: 0. 25 um; Data type: Kovats RI; Authors: Sojak, L.; Ruman, J.; J

Characterization of Monoalkylcyclopentadiens by Retention-Structure Co

in Capillary Gas Chromatography, J. Chromatogr., 391, 1987, 79-87.)NIST

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- **Retention Index (Normal Alkane):**

659. 3 (Program type: Complex; Column... (show more)class: Standard n

Column diameter: 0. 1 mm; Column length: 20 m; Column type: Capillary

Description: 40C(0. 4min) => 10C/min=> 110C=> 20C/min => 260C (1

CAS no: 96399; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. .

Data type: Normal alkane RI; Authors: LECO Corporation, Rapid qualitativ

GC/TOFMS analysis of unleaded gasoline, 2003.)NIST Spectranist ri

638. 8 (Program type: Complex; Column... (show more)class: Standard n

Column diameter: 0. 1 mm; Column length: 20 m; Column type: Capillary

Description: 40C(0. 4min) => 10C/min => 110C => 20C/min => 260C (

CAS no: 96399; Active phase: DB-1; Carrier gas: He; Phase thickness: 0. .

Data type: Normal alkane RI; Authors: LECO Corporation, Rapid qualitativ

GC/TOFMS analysis of a petroleum refinery reformat standard, 2003.)NI

Spectranist ri

626 (Program type: Ramp; Column cl... (show more)ass: Semi-standard n

polar; Column type: Capillary; CAS no: 96399; Active phase: Squalane; D
Normal alkane RI; Authors: Chen, H.-F., Quantitative prediction of gas
chromatography retention indices with support vector machines, radial b
neutral networks and multiple linear regression, Anal. Chim. Acta, 609, 2
36.)NIST Spectranist ri

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

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) = 2.80
Boiling 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 C VP (exp database): 1.24E+02 mm
Hg at 25 deg C Water Solubility Estimate from Log Kow (WSKOW v1.41): Water
Solubility at 25 deg C (mg/L): 153.7 log Kow used: 2.80 (estimated) no-
melting pt equation used Water Sol Estimate from Fragments: Wat Sol (v1.01
est) = 1102.8 mg/L ECOSAR Class Program (ECOSAR v0.99h): Class(es) found:
Neutral Organics Henrys Law Constant (25 deg C) [HENRYWIN v3.10]: Bond Method
: 9.96E-002 atm-m³/mole Group Method: 1.17E-002 atm-m³/mole Henrys LC
[VP/WSol estimate using EPI values]: 8.780E-002 atm-m³/mole Log Octanol-Air

<https://assignbuster.com/methylcyclopentadiene-c6h8-structure/>

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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