

# [1,2,3,4,5,6,7,8-octahydrophenanthrene c14h18 structure](https://assignbuster.com/12345678-octahydrophenanthrene-c14h18-structure/)

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* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 14 H 18  |
| Average mass  | 186. 293 Da  |
| Density  | 1. 0±0. 1 g/cm 3  |
| Boiling Point  | 295. 0±0. 0 °C at 760 mmHg  |
| Flash Point  | 132. 2±14. 5 °C  |
| Molar Refractivity  | 59. 8±0. 3 cm 3  |
| Polarizability  | 23. 7±0. 5 10 -24 cm 3  |
| Surface Tension  | 39. 8±3. 0 dyne/cm  |
| Molar Volume  | 183. 1±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 16. 7 °CJean-Claude Bradley Open Melting Point Dataset24097  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1652 (estimated with error: 55)NIST Spectramainlib\_229766, replib\_27673, replib\_157405  |
| 1716 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 5 mm; Column length: 100 m; Column type: Capillary; Start T: 175 C; CAS no: 5325973; Active phase: SE-30; Data type: Kovats RI; Authors: Bredael, P., Retention indices of hydrocarbons on SE-30, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 5, 1982, 325-328.)NIST Spectranist ri  |
| 1694 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Packed; Start T: 150 C; CAS no: 5325973; Active phase: SE-30; Data type: Kovats RI; Authors: Shlyakhov, A. F.; Anvaer, B. I.; Zolotareva, O. V.; Romina, N. N.; Novikova, N. V.; Koreshkova, R. I., On the possibility of group indentification of hydrocarbons by gas chromatography from temperature coefficients of retention indices, Zh. Anal. Khim., 30, 1975, 788-792.)NIST Spectranist ri  |
| 1731 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Packed; Start T: 200 C; CAS no: 5325973; Active phase: SE-30; Data type: Kovats RI; Authors: Shlyakhov, A. F.; Anvaer, B. I.; Zolotareva, O. V.; Romina, N. N.; Novikova, N. V.; Koreshkova, R. I., On the possibility of group indentification of hydrocarbons by gas chromatography from temperature coefficients of retention indices, Zh. Anal. Khim., 30, 1975, 788-792.)NIST Spectranist ri  |
| 1765 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 150 C; CAS no: 5325973; Active phase: Apiezon L; Data type: Kovats RI; Authors: Shlyakhov, A. F.; Anvaer, B. I.; Zolotareva, O. V.; Romina, N. N.; Novikova, N. V.; Koreshkova, R. I., On the possibility of group indentification of hydrocarbons by gas chromatography from temperature coefficients of retention indices, Zh. Anal. Khim., 30, 1975, 788-792.)NIST Spectranist ri  |

## Retention Index (Lee):

|  |
| --- |
| 292. 3 (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: 50 C; End T: 300 C; CAS no: 5325973; Active phase: DB-5; Phase thickness: 0. 25 um; Data type: Lee RI; Authors: Durlak, S. K.; Biswas, P.; Shi, J.; Bernhard, M. J., Characterization of polycyclic aromatic hydrocarbon particulate and gaseous emissions from polystyrene combustion, Environ. Sci. Technol., 32, 1998, 2301-2307.)NIST Spectranist ri  |
| 291. 63 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 22 mm; Column length: 20 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 50 C; End T: 300 C; CAS no: 5325973; Active phase: SE-54; Carrier gas: He; Phase thickness: 0. 20 um; Data type: Lee RI; Authors: Guillen, M. D.; Blanco, J.; Bermejo, J.; Blanco, C. G., Temperature programmed retention indices of some PAHs on Capillary columns coated with OV-1701 and SE-54, J. Hi. Res. Chromatogr., 12, 1989, 552-554.)NIST Spectranist ri  |
| 291. 4 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 5325973; Active phase: SE-52; Data type: Lee RI; Authors: Shlyakhov, A. F., Gas chromatography in organic geochemistry, Nedra, Moscow, 1984, 221.)NIST Spectranist ri  |
| 292. 03 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 3 mm; Column length: 12 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 250 C; CAS no: 5325973; Active phase: SE-52; Carrier gas: He; Phase thickness: 0. 34 um; Data type: Lee RI; Authors: Lee, M. L.; Vassilaros, D. L.; White, C. M.; Novotny, M., Retention Indices for Programmed-Temperature Capillary-Column Gas Chromatography of Polycyclic Aromatic Hydrocarbons, Anal. Chem., 51(6), 1979, 768-773., Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column type: Capillary; CAS no: 5325973; Active phase: SE-52; Data type: Lee RI; Authors: Shlyakhov, A. F., Gas chromatography in organic geochemistry, Nedra, Moscow, 1984, 221.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1696 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Heat rate: 3 K/min; Start T: 60 C; End T: 300 C; End time: 35 min; CAS no: 5325973; Active phase: Ultra-1; Carrier gas: H2; Phase thickness: 0. 33 um; Data type: Normal alkane RI; Authors: Elizalde-Gonzalez, M. P.; Hutfliess, M.; Hedden, K., Retention index system, adsorption characteristics, and sructure correlations of polycyclic aromatic hydrocarbons in fuels, J. Hi. Res. Chromatogr., 19, 1996, 345-352.)NIST Spectranist ri  |
| 1720 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Packed; Start T: 183 C; CAS no: 5325973; Active phase: Polydimethyl siloxane; Data type: Normal alkane RI; Authors: Ferrand, R., Gas phase chromatography using retention indices for the analysis of tars and their hydrogenation products, Journees internationales d’etude des methodes de separation immediate at de chromatographie; Org. sur l’initiative du IX., , 1962, 132-140.)NIST Spectranist ri  |

## Retention Index (Linear):

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| --- |
| 1705. 5 (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: 2 K/min; Start T: 40 C; End T: 310 C; CAS no: 5325973; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c. and g. c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10), 1995, 1436-1451., 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: 2 K/min; Start T: 40 C; End T: 310 C; CAS no: 5325973; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed retention indices for GC and GC-MS of hydrocarbon fuels and simulated distillation GC of heavy oils, in Analytical advances for hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publishers, New York, 2003, 147-193.)NIST Spectranist ri  |
| 1721. 1 (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: 4 K/min; Start T: 40 C; End T: 310 C; CAS no: 5325973; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c. and g. c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10), 1995, 1436-1451., 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: 4 K/min; Start T: 40 C; End T: 310 C; CAS no: 5325973; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed retention indices for GC and GC-MS of hydrocarbon fuels and simulated distillation GC of heavy oils, in Analytical advances for hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publishers, New York, 2003, 147-193.)NIST Spectranist ri  |
| 1730. 6 (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: 40 C; End T: 310 C; CAS no: 5325973; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c. and g. c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10), 1995, 1436-1451., 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: 40 C; End T: 310 C; CAS no: 5325973; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed retention indices for GC and GC-MS of hydrocarbon fuels and simulated distillation GC of heavy oils, in Analytical advances for hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publishers, New York, 2003, 147-193.)NIST Spectranist ri  |
| 1693 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 50 mm; Column length: 33. 3 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; End T: 320 C; Start time: 5 min; CAS no: 5325973; Active phase: SE-52; Carrier gas: He; Data type: Linear RI; Authors: Beernaert, H., Gas Chromatographic Analysis of Polyclylic Aromatic Hydrocarbons, J. Chromatogr., 173, 1979, 109-118.)NIST Spectranist ri  |

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

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| --- | --- |
| Density:  | 1. 0±0. 1 g/cm 3  |
| Boiling Point:  | 295. 0±0. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 3 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 51. 3±0. 8 kJ/mol  |
| Flash Point:  | 132. 2±14. 5 °C  |
| Index of Refraction:  | 1. 567  |
| Molar Refractivity:  | 59. 8±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  | 1  |

|  |  |
| --- | --- |
| ACD/LogP:  | 5. 59  |
| ACD/LogD (pH 5. 5):  | 5. 09  |
| ACD/BCF (pH 5. 5):  | 4342. 43  |
| ACD/KOC (pH 5. 5):  | 13979. 21  |
| ACD/LogD (pH 7. 4):  | 5. 09  |
| ACD/BCF (pH 7. 4):  | 4342. 43  |
| ACD/KOC (pH 7. 4):  | 13979. 21  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 23. 7±0. 5 10 -24 cm 3  |
| Surface Tension:  | 39. 8±3. 0 dyne/cm  |
| Molar Volume:  | 183. 1±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) = 5. 09Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 275. 18 (Adapted Stein & Brown method)Melting Pt (deg C): 46. 90 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00785 (Modified Grain method)Subcooled liquid VP: 0. 0125 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): 0. 6687log Kow used: 5. 09 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 4. 8432 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 08E-001 atm-m3/moleGroup Method: 6. 14E-004 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 878E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 09 (KowWin est)Log Kaw used: 0. 930 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 160Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6589Biowin2 (Non-Linear Model) : 0. 5898Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7875 (weeks )Biowin4 (Primary Survey Model) : 3. 5790 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3343Biowin6 (MITI Non-Linear Model): 0. 2942Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 3446Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 1. 7617BioHC Half-Life (days) : 57. 7683Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 1. 67 Pa (0. 0125 mm Hg)Log Koa (Koawin est ): 4. 160Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 8E-006 Octanol/air (Koa) model: 3. 55E-009 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 6. 5E-005 Mackay model : 0. 000144 Octanol/air (Koa) model: 2. 84E-007 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 255. 0644 E-12 cm3/molecule-secHalf-Life = 0. 042 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 503 HrsOzone Reaction: OVERALL Ozone Rate Constant = 410. 844971 E-17 cm3/molecule-secHalf-Life = 0. 003 Days (at 7E11 mol/cm3)Half-Life = 4. 017 MinFraction sorbed to airborne particulates (phi): 0. 000104 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 5586Log Koc: 3. 747 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 = 3. 220 (BCF = 1660)log Kow used: 5. 09 (estimated)Volatilization from Water: Henry LC: 0. 000614 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 2. 694 hoursHalf-Life from Model Lake : 143. 8 hours (5. 993 days)Removal In Wastewater Treatment: Total removal: 81. 73 percentTotal biodegradation: 0. 66 percentTotal sludge adsorption: 77. 50 percentTotal to Air: 3. 57 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 00796 0. 0628 1000 Water 13. 4 360 1000 Soil 68 720 1000 Sediment 18. 5 3. 24e+003 0 Persistence Time: 508 hr

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* 1-Click Scaffold Hop