

# [2-methyl-1-octene c9h18 structure](https://assignbuster.com/2-methyl-1-octene-c9h18-structure/)

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* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 9 H 18  |
| Average mass  | 126. 239 Da  |
| Density  | 0. 7±0. 1 g/cm 3  |
| Boiling Point  | 142. 6±7. 0 °C at 760 mmHg  |
| Flash Point  | 26. 9±2. 4 °C  |
| Molar Refractivity  | 43. 3±0. 3 cm 3  |
| Polarizability  | 17. 2±0. 5 10 -24 cm 3  |
| Surface Tension  | 22. 7±3. 0 dyne/cm  |
| Molar Volume  | 172. 0±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -78 °CJean-Claude Bradley Open Melting Point Dataset13607  |
| -77. 8 °CJean-Claude Bradley Open Melting Point Dataset24040  |

## Experimental Boiling Point:

|  |
| --- |
| 141-143 °CSynQuest78519, 1300-1-30  |

## Experimental Flash Point:

|  |
| --- |
| 32 °CSynQuest78519, 1300-1-30  |

## Experimental Gravity:

|  |
| --- |
| 0. 74 g/mLSynQuest1300-1-30  |

* Miscellaneous

## Safety:

|  |
| --- |
| FlammableSynQuest1300-1-30, 78519  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 883 (estimated with error: 39)NIST Spectramainlib\_227609, replib\_2463, replib\_155943  |
| 860 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 2 mm; Column length: 100 m; Column type: Capillary; Description: 5C(10min)=> 5C/min=> 50C(48min)=> 1. 5C/min=> 195C(91min); CAS no: 4588185; Active phase: Petrocol DH-100; Carrier gas: He; Data type: Kovats RI; Authors: Haagen-Smit Laboratory, Procedure for the detailed hydrocarbon analysis of gasolines by single column high efficiency (capillary) column gas chromatography, SOP NO. MLD 118, Revision No. 1. 1, California Environmental Protection Agency, Air Resources Board, El Monte, California, 1997, 22.)NIST Spectranist ri  |
| 880 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 40 C; CAS no: 4588185; Active phase: OV-101; Data type: Kovats RI; Authors: Laub, R. J.; Purnell, J. H., Specific retention volumes, retention indices, and family-plot regressions of aliphatic, alicyclic, and aromatic hydrocarbon solutes with OV-101 poly (dimethylsiloxane) stationary phase, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 11, 1988, 649-660.)NIST Spectranist ri  |
| 881 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 60 C; CAS no: 4588185; Active phase: OV-101; Data type: Kovats RI; Authors: Laub, R. J.; Purnell, J. H., Specific retention volumes, retention indices, and family-plot regressions of aliphatic, alicyclic, and aromatic hydrocarbon solutes with OV-101 poly (dimethylsiloxane) stationary phase, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 11, 1988, 649-660.)NIST Spectranist ri  |
| 882 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 80 C; CAS no: 4588185; Active phase: OV-101; Data type: Kovats RI; Authors: Laub, R. J.; Purnell, J. H., Specific retention volumes, retention indices, and family-plot regressions of aliphatic, alicyclic, and aromatic hydrocarbon solutes with OV-101 poly (dimethylsiloxane) stationary phase, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 11, 1988, 649-660.)NIST Spectranist ri  |
| 874 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 120 m; Column type: Capillary; Start T: 100 C; CAS no: 4588185; Active phase: Squalane; Carrier gas: He; Data type: Kovats RI; Authors: Lulova, N. I.; Leont’eva, S. A.; Timofeeva, A. N., Gas-chromatographic method of determination of individual hydrocarbons in catalytic cracking gasolines, in Proceedings of All-Union Research Institute on Oil Processes. Vol. 18, All-Union Research Institute on Oil Processes, Moscow, 1976, 30-53., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 120 m; Column type: Capillary; Start T: 55 C; CAS no: 4588185; Active phase: Squalane; Carrier gas: He; Data type: Kovats RI; Authors: Lulova, N. I.; Leont’eva, S. A.; Fedosova, A. K.; Kvasova, V. A., Individual composition of hydrocarbons in naphthas from secondary processes, Chem. Technol. Fuels Oils (Engl. Transl.), 11(1/2), 1975, 59-64., Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column length: 100 m; Column type: Capillary; Start T: 80 C; CAS no: 4588185; Active phase: Squalane; Carrier gas: Ar; Data type: Kovats RI; Authors: Schomburg, G., Struktur und Retentionsverhalten von Offenkettigen und Cyclischen Kohlenwasserstoffen und Deren Einfacher Substitutionsprodukte, Anal. Chim. Acta., 38, 1967, 45-64.)NIST Spectranist ri  |
| 868 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 2 mm; Column length: 50 m; Column type: Capillary; Start T: 100 C; CAS no: 4588185; Active phase: Squalane; Carrier gas: H2; Data type: Kovats RI; Authors: Mitra, G. D.; Mohan, G.; Sinha, A., Gas chromatographic analysis of complex hydrocarbon mixtures, J. Chromatogr. A, 91, 1974, 633-648.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 876 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 35 C; End T: 200 C; End time: 10 min; Start time: 15 min; CAS no: 4588185; Active phase: PONA; Carrier gas: Nitrogen; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Zhang, X.; Ding, L.; Sun, Z.; Song, L.; Sun, T., Study on quantitative structure-retention relationships for hydrocarbons in FCC gasoline, Chromatographia, 70(3/4), 2009, 511-518.)NIST Spectranist ri  |
| 880 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 20 mm; Column length: 50 m; Column type: Capillary; Heat rate: 1 K/min; Start T: 30 C; End T: 100 C; Start time: 6 min; CAS no: 4588185; Active phase: OV-101; Carrier gas: Helium; Phase thickness: 0. 50 um; Data type: Normal alkane RI; Authors: Orav, A.; Kailas, T.; Muurisepp, M.; Kann, J., Composition of the oil from waste tires. 1. Fraction boiling at yp to 160 0C, Proc. Estonian Acad. Sci. Chem., 48(1), 1999, 30-39.)NIST Spectranist ri  |
| 898 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; CAS no: 4588185; Active phase: DB-1; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Ciccioli, P.; Cecinato, A.; Brancaleoni, E.; Brachetti, A.; Frattoni, M.; Sparapani, R., Composition and Distribution of Polar and Non-Polar VOCs in Urban, Rural, Forest and Remote Areas, Eur Commission EUR, , 1994, 549-568.)NIST Spectranist ri  |
| 874 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 70 C; CAS no: 4588185; Active phase: Squalane; Data type: Normal alkane RI; Authors: Schomburg, G., Gaschromatographische Retentionsdaten und Struktur Chemischer Verbindungen. II. Methylverzweigungen und Doppelbindungen in Offenkettigen Kohlenwasserstoffen, J. Chromatogr., 23, 1966, 1-17.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 881 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 25 mm; Column length: 100 m; Column type: Capillary; Heat rate: 1 K/min; Start T: 30 C; End T: 220 C; CAS no: 4588185; Active phase: Petrocol DH; Carrier gas: He; Phase thickness: 0. 5 um; Data type: Linear RI; Authors: White, C. M.; Hackett, J.; Anderson, R. R.; Kail, S.; Spock, P. S., Linear temperature programmed retention indices of gasoline range hydrocarbons and chlorinated hydrocarbons on cross-linked polydimethylsiloxane, J. Hi. Res. Chromatogr., 15, 1992, 105-120.)NIST Spectranist ri  |
| 883 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 30C=> 5K/min= 120C=> 10C/min=> 270C; CAS no: 4588185; Active phase: DB-5; Carrier gas: He; Data type: Linear RI; Authors: Zaikin, V. G.; Borisov, R. S., Chromatographic-mass spectrometric analysis of Fishcer-Tropsch synthesis products, J. Anal. Chem. USSR (Engl. Transl.), 57(6), 2002, 544-551, In original 653-660.)NIST Spectranist ri  |

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

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| --- | --- |
| Density:  | 0. 7±0. 1 g/cm 3  |
| Boiling Point:  | 142. 6±7. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 6. 9±0. 1 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 36. 4±0. 8 kJ/mol  |
| Flash Point:  | 26. 9±2. 4 °C  |
| Index of Refraction:  | 1. 418  |
| Molar Refractivity:  | 43. 3±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 5  |
| #Rule of 5 Violations:  | 1  |

|  |  |
| --- | --- |
| ACD/LogP:  | 5. 05  |
| ACD/LogD (pH 5. 5):  | 4. 49  |
| ACD/BCF (pH 5. 5):  | 1526. 22  |
| ACD/KOC (pH 5. 5):  | 6613. 51  |
| ACD/LogD (pH 7. 4):  | 4. 49  |
| ACD/BCF (pH 7. 4):  | 1526. 22  |
| ACD/KOC (pH 7. 4):  | 6613. 51  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 17. 2±0. 5 10 -24 cm 3  |
| Surface Tension:  | 22. 7±3. 0 dyne/cm  |
| Molar Volume:  | 172. 0±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. 68Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 134. 86 (Adapted Stein & Brown method)Melting Pt (deg C): -66. 30 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 6. 46 (Mean VP of Antoine & Grain methods)MP (exp database): -77. 8 deg CBP (exp database): 144. 8 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 2. 776log Kow used: 4. 68 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 2. 1226 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 9. 90E-001 atm-m3/moleGroup Method: 1. 58E+000 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 3. 865E-001 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 68 (KowWin est)Log Kaw used: 1. 607 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 3. 073Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7959Biowin2 (Non-Linear Model) : 0. 9552Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 2185 (weeks )Biowin4 (Primary Survey Model) : 3. 9347 (days )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5968Biowin6 (MITI Non-Linear Model): 0. 7548Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 3421Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 0. 6147BioHC Half-Life (days) : 4. 1184Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 793 Pa (5. 95 mm Hg)Log Koa (Koawin est ): 3. 073Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 78E-009 Octanol/air (Koa) model: 2. 9E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 37E-007 Mackay model : 3. 03E-007 Octanol/air (Koa) model: 2. 32E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 58. 2401 E-12 cm3/molecule-secHalf-Life = 0. 184 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 2. 204 HrsOzone Reaction: OVERALL Ozone Rate Constant = 1. 200000 E-17 cm3/molecule-secHalf-Life = 0. 955 Days (at 7E11 mol/cm3)Half-Life = 22. 920 HrsFraction sorbed to airborne particulates (phi): 2. 2E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 783. 4Log Koc: 2. 894 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. 904 (BCF = 802. 5)log Kow used: 4. 68 (estimated)Volatilization from Water: Henry LC: 0. 99 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 147 hoursHalf-Life from Model Lake : 106. 7 hours (4. 447 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 99. 81 percentTotal biodegradation: 0. 12 percentTotal sludge adsorption: 39. 40 percentTotal to Air: 60. 29 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 2. 93 3. 7 1000 Water 45. 1 360 1000 Soil 26. 3 720 1000 Sediment 25. 7 3. 24e+003 0 Persistence Time: 135 hr

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