

# [3-methyl-2-ethyl-1-butene c7h14 structure](https://assignbuster.com/3-methyl-2-ethyl-1-butene-c7h14-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 7 H 14  |
| Average mass  | 98. 186 Da  |
| Density  | 0. 7±0. 1 g/cm 3  |
| Boiling Point  | 85. 1±7. 0 °C at 760 mmHg  |
| Flash Point  | -10. 5±8. 1 °C  |
| Molar Refractivity  | 34. 0±0. 3 cm 3  |
| Polarizability  | 13. 5±0. 5 10 -24 cm 3  |
| Surface Tension  | 19. 6±3. 0 dyne/cm  |
| Molar Volume  | 139. 4±3. 0 cm 3  |

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

## Retention Index (Kovats):

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| --- |
| 620 (estimated with error: 39)NIST Spectramainlib\_912  |
| 665. 8 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 250 um; Column length: 150 m; Column type: Capillary; Start T: 30 C; CAS no: 7357939; Active phase: Methyl Silicone; Carrier gas: He; Data type: Kovats RI; Authors: Sojak, L.; Addova, G.; Kubinec, R.; Kraus, A.; Hu, G., Gas chromatographic-mass spectrometric characterization of all acyclic C5-C7 alkenes from fluid catalytic cracked gasoline using polydimethylsiloxane and squalane stationary phases, J. Chromatogr. A, 947, 2002, 103-117.)NIST Spectranist ri  |
| 662. 7 (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: 7357939; 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  |
| 666 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 21 mm; Column length: 50 m; Column type: Capillary; Start T: 40 C; CAS no: 7357939; Active phase: HP-PONA; Carrier gas: H2; Phase thickness: 0. 5 um; Data type: Kovats RI; Authors: Lubeck, A. J.; Sutton, D. L., Kovats Retention Indices of Selected Olefins on Bonded Phase Fused Silica Capillaries, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 7(9), 1984, 542-544., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 264 mm; Column length: 60 m; Column type: Capillary; Start T: 40 C; CAS no: 7357939; Active phase: DB-1; Carrier gas: H2; Phase thickness: 0. 25 um; Data type: Kovats RI; Authors: Lubeck, A. J.; Sutton, D. L., Kovats Retention Indices of Selected Olefins on Bonded Phase Fused Silica Capillaries, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 7(9), 1984, 542-544.)NIST Spectranist ri  |
| 658. 3 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 250 um; Column length: 93 m; Column type: Capillary; Start T: 30 C; CAS no: 7357939; Active phase: Squalane; Carrier gas: He; Data type: Kovats RI; Authors: Sojak, L.; Addova, G.; Kubinec, R.; Kraus, A.; Hu, G., Gas chromatographic-mass spectrometric characterization of all acyclic C5-C7 alkenes from fluid catalytic cracked gasoline using polydimethylsiloxane and squalane stationary phases, J. Chromatogr. A, 947, 2002, 103-117.)NIST Spectranist ri  |
| 659 (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: 7357939; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Rijks, J. A.; Cramers, C. A., High precision capillary gas chromatography of hydrocarbons, Chromatographia, 7(3), 1974, 99-106., 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: 7357939; 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 type: Capillary; Start T: 50 C; CAS no: 7357939; Active phase: Squalane; Data type: Kovats RI; Authors: Chretien, J. R.; Dubois, J.-E., New Perspectives in the Prediction of Kovats Indices, J. Chromatogr., 126, 1976, 171-189.)NIST Spectranist ri  |
| 660 (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: 70 C; CAS no: 7357939; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Rijks, J. A.; Cramers, C. A., High precision capillary gas chromatography of hydrocarbons, Chromatographia, 7(3), 1974, 99-106., 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: 7357939; 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 ft; Column type: Packed; Start T: 67 C; CAS no: 7357939; 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  |
| 662 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 300 ft; Column type: Capillary; Start T: 40 C; CAS no: 7357939; Active phase: Squalane; Carrier gas: N2; Data type: Kovats RI; Authors: Matukuma, A., Retention indices of alkanes through C10 and alkenes through C8 and relation between boiling points and retention data, Gas Chromatogr., Int. Symp. Anal. Instrum. Div Instrum Soc. Amer., 7, 1969, 55-75.)NIST Spectranist ri  |
| 661 (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: 86 C; CAS no: 7357939; 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  |

## Retention Index (Normal Alkane):

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| 652 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capillary; Heat rate: 2 K/min; Start T: -20 C; CAS no: 7357939; Active phase: DB-1; Carrier gas: He; Phase thickness: 1. 0 um; Data type: Normal alkane RI; Authors: Ramnas, O.; Ostermark, U.; Peterson, G., Characterization of sixty alkenes in a cat-cracked gasoline naphtha by gas chromatography, Chromatographia, 38(3/4), 1994, 222-226.)NIST Spectranist ri  |
| 659 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 28 mm; Column length: 74. 6 m; Column type: Capillary; Start T: 50 C; CAS no: 7357939; Active phase: Methyl Silicone; Carrier gas: N2; Data type: Normal alkane RI; Authors: Xu, Y., Capillary gas chromatographic analysis of individual hydrocarbons in catalytic cracking gasoline boiling below 100 C, Chin. J. Chromatogr., 7(2), 1989, 88-92.)NIST Spectranist ri  |
| 658. 6 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 93 m; Column type: Capillary; Start T: 40 C; CAS no: 7357939; Active phase: Squalane; Carrier gas: He; Data type: Normal alkane RI; Authors: Sojak, L.; Addova, G.; Kubinec, R.; Ruman, J.; Hu, G., GC-MS characterization of all acyclic C5-C7 alkenes from FCC gasoline using squalane stationary phase, Petroleum and Coal, 42(3-4), 2000, 188-194.)NIST Spectranist ri  |
| 658 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 70 C; CAS no: 7357939; 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):

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| --- |
| 667. 6 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 250 um; Column length: 150 m; Column type: Capillary; Heat rate: 1 K/min; Start T: 30 C; End T: 200 C; CAS no: 7357939; Active phase: Methyl Silicone; Carrier gas: He; Data type: Linear RI; Authors: Sojak, L.; Addova, G.; Kubinec, R.; Kraus, A.; Hu, G., Gas chromatographic-mass spectrometric characterization of all acyclic C5-C7 alkenes from fluid catalytic cracked gasoline using polydimethylsiloxane and squalane stationary phases, J. Chromatogr. A, 947, 2002, 103-117.)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:  | 85. 1±7. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 78. 8±0. 1 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 31. 2±0. 8 kJ/mol  |
| Flash Point:  | -10. 5±8. 1 °C  |
| Index of Refraction:  | 1. 403  |
| Molar Refractivity:  | 34. 0±0. 3 cm 3  |
| #H bond acceptors:  | 0  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 2  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 3. 80  |
| ACD/LogD (pH 5. 5):  | 3. 52  |
| ACD/BCF (pH 5. 5):  | 277. 64  |
| ACD/KOC (pH 5. 5):  | 1952. 78  |
| ACD/LogD (pH 7. 4):  | 3. 52  |
| ACD/BCF (pH 7. 4):  | 277. 64  |
| ACD/KOC (pH 7. 4):  | 1952. 78  |
| Polar Surface Area:  | 0 Å 2  |
| Polarizability:  | 13. 5±0. 5 10 -24 cm 3  |
| Surface Tension:  | 19. 6±3. 0 dyne/cm  |
| Molar Volume:  | 139. 4±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) = 3. 63Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 72. 78 (Adapted Stein & Brown method)Melting Pt (deg C): -103. 20 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 67. 4 (Mean VP of Antoine & Grain methods)BP (exp database): 89 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 27. 55log Kow used: 3. 63 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 32. 811 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 62E-001 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 3. 161E-001 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 63 (KowWin est)Log Kaw used: 1. 361 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 2. 269Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7008Biowin2 (Non-Linear Model) : 0. 8340Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 9822 (weeks )Biowin4 (Primary Survey Model) : 3. 7061 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4324Biowin6 (MITI Non-Linear Model): 0. 5340Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 3105Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 0. 5432BioHC Half-Life (days) : 3. 4932Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 8. 65E+003 Pa (64. 9 mm Hg)Log Koa (Koawin est ): 2. 269Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 47E-010 Octanol/air (Koa) model: 4. 56E-011 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 25E-008 Mackay model : 2. 77E-008 Octanol/air (Koa) model: 3. 65E-009 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 54. 7758 E-12 cm3/molecule-secHalf-Life = 0. 195 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 2. 343 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. 01E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 206. 4Log Koc: 2. 315 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. 092 (BCF = 123. 5)log Kow used: 3. 63 (estimated)Volatilization from Water: Henry LC: 0. 562 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 012 hoursHalf-Life from Model Lake : 94. 13 hours (3. 922 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 99. 57 percentTotal biodegradation: 0. 04 percentTotal sludge adsorption: 8. 89 percentTotal to Air: 90. 64 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 5. 69 3. 89 1000 Water 80. 8 360 1000 Soil 8. 81 720 1000 Sediment 4. 69 3. 24e+003 0 Persistence Time: 76 hr

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