

3-methyl-2-ethyl-1-  
butene  $C_7H_{14}$   
structure



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## Contents

- Retention Index (Linear):

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

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

- **Retention Index (Kovats):**

620 (estimated with error: 39)NIST Spectramainlib\_912

665. 8 (Program type: Isothermal; Col... (show more)umn class: Standard n...  
polar; Column diameter: 250 um; Column length: 150 m; Column type: C...  
Start T: 30 C; CAS no: 7357939; Active phase: Methyl Silicone; Carrier ga...  
Data type: Kovats RI; Authors: Sojak, L.; Addova, G.; Kubinec, R.; Kraus, A...  
G., Gas chromatographic-mass spectrometric characterization of all acyclo...  
alkenes from fluid catalytic cracked gasoline using polydimethylsiloxane...  
squalane stationary phases, J. Chromatogr. A, 947, 2002, 103-117.)NIST...  
Spectranist ri

662. 7 (Program type: Complex; Column... (show more)class: Standard n...  
Column diameter: 0. 2 mm; Column length: 100 m; Column type: Capilla...  
Description: 5C(10min)=> 5C/min=> 50C(48min)=> 1. 5C/min=> 195C...  
CAS no: 7357939; Active phase: Petrocol DH-100; Carrier gas: He; Data t...  
Kovats RI; Authors: Haagen-Smit Laboratory, Procedure for the detailed...  
hydrocarbon analysis of gasolines by single column high efficiency (capil...  
column gas chromatography, SOP NO. MLD 118, Revision No. 1. 1, Califo...  
Environmental Protection Agency, Air Resources Board, El Monte, Californi...  
1997, 22.)NIST Spectranist ri

666 (Program type: Isothermal; Col... (show more)umn class: Standard n...  
Column diameter: 0. 21 mm; Column length: 50 m; Column type: Capilla...  
T: 40 C; CAS no: 7357939; Active phase: HP-PONA; Carrier gas: H2; Phas...  
thickness: 0. 5 um; Data type: Kovats RI; Authors: Lubeck, A. J.; Sutton, D...  
Kovats Retention Indices of Selected Olefins on Bonded Phase Fused Silic...

Capillaries, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 7(9), 1984, 54  
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,  
Kovats Retention Indices of Selected Olefins on Bonded Phase Fused Silica  
Capillaries, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 7(9), 1984, 54  
544.)NIST Spectranist ri

658. 3 (Program type: Isothermal; Col... (show more)umn class: Semi-stationary  
non-polar; Column diameter: 250 um; Column length: 93 m; Column type:  
Capillary; Start T: 30 C; CAS no: 7357939; Active phase: Squalane; Carrier  
He; Data type: Kovats RI; Authors: Sojak, L.; Addova, G.; Kubinec, R.; Kra  
Hu, G., Gas chromatographic-mass spectrometric characterization of all  
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-stationary  
polar; Column diameter: 0.25 mm; Column length: 100 m; Column type:  
Capillary; Start T: 50 C; CAS no: 7357939; Active phase: Squalane; Carrier  
N2; Data type: Kovats RI; Authors: Rijks, J. A.; Cramers, C. A., High precision  
capillary gas chromatography of hydrocarbons, Chromatographia, 7(3), 1974,  
106., Program type: Isothermal; Col... (show more)umn class: Semi-stationary  
polar; Column diameter: 0.25 mm; Column length: 50 ft; Column type: P  
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; Column class: Semi-standard non-polar; Column type: Capillary; Start T: 67 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 Retention Indices, J. Chromatogr., 126, 1976, 171-189.)NIST Spectranist ri

660 (Program type: Isothermal; Column 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), 1968, 106., Program type: Isothermal; Column 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; Column 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-stand  
polar; Column diameter: 0. 25 mm; Column length: 300 ft; Column type:  
Capillary; Start T: 40 C; CAS no: 7357939; Active phase: Squalane; Carrie  
N2; Data type: Kovats RI; Authors: Matukuma, A., Retention indices of alk  
through C10 and alkenes through C8 and relation between boiling points  
retention data, Gas Chromatogr., Int. Symp. Anal. Instrum. Div Instrum S  
Amer., 7, 1969, 55-75.)NIST Spectranist ri

661 (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: 86 C; CAS no: 7357939; Active phase: Squalane; Carrier gas: He;  
Substrate: Chromosorb P; Data type: Kovats RI; Authors: Hively, R. A.; Hi  
E., Variation of the retention index with temperature on squalane substra  
Gas Chromatogr., 6, 1968, 203-217.)NIST Spectranist ri

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

652 (Program type: Ramp; Column cl... (show more)ass: Standard non-po  
Column diameter: 0. 32 mm; Column length: 50 m; Column type: Capilla  
rate: 2 K/min; Start T: -20 C; CAS no: 7357939; Active phase: DB-1; Carri  
He; Phase thickness: 1. 0 um; Data type: Normal alkane RI; Authors: Ram  
Ostermark, U.; Peterson, G., Characterization of sixty alkenes in a cat-cra  
gasoline naphtha by gas chromatography, Chromatographia, 38(3/4), 19  
226.)NIST Spectranist ri

659 (Program type: Isothermal; Col... (show more)umn class: Standard n  
Column diameter: 0. 28 mm; Column length: 74. 6 m; Column type: Capi  
Start T: 50 C; CAS no: 7357939; Active phase: Methyl Silicone; Carrier ga

Data type: Normal alkane RI; Authors: Xu, Y., Capillary gas chromatography analysis of individual hydrocarbons in catalytic cracking gasoline boiling 100 C, Chin. J. Chromatogr., 7(2), 1989, 88-92.)NIST Spectranist ri

658. 6 (Program type: Isothermal; Col... (show more)umn class: Semi-sta non-polar; Column diameter: 0. 25 mm; Column length: 93 m; Column ty Capillary; Start T: 40 C; CAS no: 7357939; Active phase: Squalane; Carrie He; Data type: Normal alkane RI; Authors: Sojak, L.; Addova, G.; Kubinec Ruman, J.; Hu, G., GC-MS characterization of all acyclic C5-C7 alkenes from gasoline using squalane stationary phase, Petroleum and Coal, 42(3-4), 2 188-194.)NIST Spectranist ri

658 (Program type: Isothermal; Col... (show more)umn class: Semi-stand polar; Column type: Capillary; Start T: 70 C; CAS no: 7357939; Active pha Squalane; Data type: Normal alkane RI; Authors: Schomburg, G., Gaschromatographische Retentionsdaten und Struktur Chemischer Verbindungen. II. Methylverzweigungen und Doppelbindungen in Offenke Kohlenwasserstoffen, J. Chromatogr., 23, 1966, 1-17.)NIST Spectranist ri

- **Retention Index (Linear):**

667. 6 (Program type: Ramp; Column cl... (show more)ass: Standard non Column diameter: 250 um; Column length: 150 m; Column type: Capillar rate: 1 K/min; Start T: 30 C; End T: 200 C; CAS no: 7357939; Active phas Silicone; Carrier gas: He; Data type: Linear RI; Authors: Sojak, L.; Addova Kubinec, R.; Kraus, A.; Hu, G., Gas chromatographic-mass spectrometric characterization of all acyclic C5-C7 alkenes from fluid catalytic cracked using polydimethylsiloxane and squalane stationary phases, J. Chromato

947, 2002, 103-117.)NIST Spectranist ri

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

Density:	0.7±0.1 g/cm <sup>3</sup>
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 <sup>3</sup>
#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

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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 <sup>2</sup>
Polarizability:	13. 5±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	19. 6±3. 0 dyne/cm
Molar Volume:	139. 4±3. 0 cm <sup>3</sup>

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

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(MITI Non-Linear Model): 0.5340 Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0.3105 Ready Biodegradability Prediction: NO Hydrocarbon Biodegradation (BioHCwin v1.01): LOG BioHC Half-Life (days) : 0.5432 BioHC Half-Life (days) : 3.4932 Sorption to aerosols (25 Dec C) [AEROWIN v1.00]: Vapor pressure (liquid/subcooled): 8.65E+003 Pa (64.9 mm Hg) Log Koa (Koawin est) : 2.269 Kp (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-sec Half-Life = 0.195 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 2.343 Hrs Ozone Reaction: OVERALL Ozone Rate Constant = 1.200000 E-17 cm3/molecule-sec Half-Life = 0.955 Days (at 7E11 mol/cm3) Half-Life = 22.920 Hrs Fraction sorbed to airborne particulates (phi): 2.01E-008 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation Soil Adsorption Coefficient (PCKOCWIN v1.66): Koc : 206.4 Log 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 hours Half-Life from Model Lake : 94.13 hours (3.922 days) Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 99.57 percent Total biodegradation: 0.04 percent Total sludge adsorption: 8.89 percent Total 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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