

2-methyl-1-octene
c₉h₁₈ structure



**ASSIGN
BUSTER**

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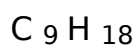
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Contents

- Retention Index (Linear):

Molecular



Formula

Average mass 126. 239 Da

Density 0. 7±0. 1 g/cm³

Boiling Point 142. 6±7. 0 °C at
760 mmHg

Flash Point 26. 9±2. 4 °C

Molar 43. 3±0. 3 cm³

Refractivity

Polarizability $17.2 \pm 0.5 \cdot 10^{-24}$
cm³

Surface 22.7 ± 3.0

Tension dyne/cm

Molar Volume 172.0 ± 3.0 cm³

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

- **Experimental Melting Point:**

-78 °C Jean-Claude

Bradley Open Melting

Point Dataset13607

-77.8 °C Jean-Claude

Bradley Open Melting

Point Dataset24040

- **Experimental Boiling Point:**

141-143

°C SynQuest78519,

1300-1-30

- **Experimental Flash Point:**

32

°CSynQuest78519,

1300-1-30

- **Experimental Gravity:**

0.74

g/mLSynQuest1300-

1-30

- Miscellaneous

- **Safety:**

FlammableSynQuest1

300-1-30, 78519

- Gas Chromatography

- **Retention Index (Kovats):**

883 (estimated with

error: 39)NIST

Spectramainlib_2276

09, 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

Substitutionsprodukt

e, 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 up 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.,

Gaschromatographisc

he 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

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 cm³

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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