Butyl isobutyrate c8h16o2 structure

\n[toc title="Table of Contents"]\n

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\n[/toc]\n \n

Contents

Molecular Formula	$C_8H_{16}O_2$
Average mass	144. 211 Da
Density	0. 9±0. 1 g/cm ^{3}
Boiling Point	156. 3±8. 0 °C at 760 mmHg
Flash Point	46. 7±8. 3 °C

Molar Refractivity	40. 8±0. 3 cm^3
Polarizability	16. 2±0. 5 10^{-24} cm^3
Surface Tension	26. 3±3. 0 dyne/cm
Molar Volume	164. 4±3. 0 cm^3

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

Experimental Melting Point:

<25

°CFooDBFDB019968

Experimental Boiling Point:

155-156 °C

(Literature)LabNetworkLN00196136

155 °CFooDBFDB019968

Experimental Flash Point:

43

°CLabNetworkLN0019613

6

- **Experimental Refraction Index:**

  20FooDBFDB0199

  68

- Gas Chromatography

  - **Retention Index (Kovats):**

    920 (estimated with error: 47)NIST Spectramainlib_4078, replib_285039,

    replib_228837, replib_249302

    935 (Program type: Ramp; Column cl... (show more)ass: Standard non-po

    Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capilla

    rate: 2 K/min; Start T: 30 C; End T: 210 C; Start time: 4 min; CAS no: 978

    Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data typ

    Kovats RI; Authors: Takeoka, G. R.; Flath, R. A.; Mon, T. R.; Teranishi, R.;

    Guentert, M., Volatile Constituents of Apricot (Prunus armeniaca), J. Agric

    Chem., 38(2), 1990, 471-477.)NIST Spectranist ri

936 (Program type: Isothermal; Col… (show more)umn class: Standard n
Column length: 3 m; Column type: Packed; Start T: 100 C; CAS no: 9787(
phase: SE-30; Carrier gas: N2; Substrate: Chromosorb W AW (60-80 mes
type: Kovats RI; Authors: Chastrette, M.; Heintz, M.; Druilhe, A.; Lefort, D
Analyse chromatographique d’esters aliphatiques satures. Relations rete
structure et prevision de la retention, Bull. Soc. Chim. Fr., , 1974, 1852-1
Program type: Ramp; Column cl… (show more)ass: Standard non-polar; C
diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat
K/min; Start T: 30 C; End T: 210 C; Start time: 4 min; CAS no: 97870; Act
phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Kova
Authors: Takeoka, G. R.; Flath, R. A.; Mon, T. R.; Teranishi, R.; Guentert, M
Volatile Constituents of Apricot (Prunus armeniaca), J. Agric. Food Chem.
1990, 471-477.)NIST Spectranist ri

943 (Program type: Ramp; Column cl… (show more)ass: Standard non-po
Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capilla
rate: 2 K/min; Start T: 30 C; End T: 210 C; Start time: 4 min; CAS no: 978
Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data typ
Kovats RI; Authors: Takeoka, G. R.; Flath, R. A.; Mon, T. R.; Teranishi, R.;
Guentert, M., Volatile Constituents of Apricot (Prunus armeniaca), J. Agric
Chem., 38(2), 1990, 471-477.)NIST Spectranist ri

944 (Program type: Ramp; Column cl… (show more)ass: Standard non-po
Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capilla
rate: 2 K/min; Start T: 30 C; End T: 210 C; Start time: 4 min; CAS no: 978
Active phase: DB-1; Carrier gas: He; Phase thickness: 0. 25 um; Data typ

Kovats RI; Authors: Takeoka, G. R.; Flath, R. A.; Mon, T. R.; Teranishi, R.; Guentert, M., Volatile Constituents of Apricot (Prunus armeniaca), J. Agric Chem., 38(2), 1990, 471-477.)NIST Spectranist ri

937 (Program type: Isothermal; Col… (show more)umn class: Standard n Column diameter: 0. 22 mm; Column length: 15 m; Column type: Capilla T: 80 C; CAS no: 97870; Active phase: OV-101; Data type: Kovats RI; Aut Komarek, K.; Hornova, L.; Horna, A.; Churacek, J., Glass capillary gas chromatography of homologous series of esters. IV. Separation of homol series of certain halogenopropyl esters of aliphatic carboxylic acids on O Chromatogr., 281, 1983, 299-303.)NIST Spectranist ri

931 (Program type: Isothermal; Col… (show more)umn class: Standard n Column length: 12 ft; Column type: Packed; Start T: 150 C; CAS no: 9787 phase: SE-30; Substrate: Celaton (62-72 mesh); Data type: Kovats RI; Au Ashes, J. R.; Haken, J. K., Gas chromatography of homologous esters. VI. Structure-retention increments of aliphatic esters, J. Chromatogr., 101, 1 103-123., Program type: Isothermal; Col… (show more)umn class: Stand polar; Column length: 12 ft; Column type: Packed; Start T: 150 C; CAS no Active phase: SE-30; Substrate: Chromosorb W AW DMCS; Data type: Ko Authors: Haken, J. K.; Srisukh, D., Gas chromatography of homologous es Molecular retention indices of aliphatic esters, J. Chromatogr., 219, 1981 Program type: Isothermal; Col… (show more)umn class: Standard non-po Column type: Capillary; CAS no: 97870; Active phase: SE-30; Data type: RI; Authors: Chretien, J. R.; Dubois, J-E., Topological Analysis: A Techniqu Physico-Chemical Exploitation of Retention Data in Gas-Liquid Chromatog

Chromatogr., 158, 1978, 43-56.)NIST Spectranist ri

933 (Program type: Isothermal; Col… (show more)umn class: Standard n
Column length: 12 ft; Column type: Packed; Start T: 150 C; CAS no: 9787
phase: SE-30; Substrate: Celite 560; Data type: Kovats RI; Authors: Germ
W.; Haken, J. K., Gas chromatography of homologous esters. Part 1. Simp
aliphatic esters, J. Chromatogr., 43, 1969, 33-42., Program type: Isotherm
Col… (show more)umn class: Standard non-polar; Column type: Packed;
150 C; CAS no: 97870; Active phase: OV-1; Data type: Kovats RI; Authors
J. R.; Haken, J. K., Gas chromatography of homologous esters. Part V. Ret
aliphatic esters on non-polar, donar and acceptor stationary phases, J.
Chromatogr., 60, 1971, 33-44.)NIST Spectranist ri

952 (Program type: Isothermal; Col… (show more)umn class: Standard n
Column length: 2 m; Column type: Packed; Start T: 100 C; CAS no: 97870
phase: SE-30; Substrate: Chromosorb W; Data type: Kovats RI; Authors: Z
D.; Chovin, P.; Guiochon, G., Identification of hydroxylic compounds and
derivatives by gas chromatography, Chromatographia, 3, 1970, 180-195
Spectranist ri

894 (Program type: Isothermal; Col… (show more)umn class: Semi-stand
polar; Column length: 2. 25 m; Column type: Packed; Start T: 130 C; CAS
97870; Active phase: Apiezon L; Substrate: Celite; Data type: Kovats RI;
Wehrli, A.; Kovats, E., Gas-chromatographische Charakterisierung ograni
Verbindungen. Teil 3: Berechnung der Retentionsindices aliphatischer,
alicyclischer und aromatischer Verbindungen, Helv. Chim. Acta, 7, 1959,
2736., Program type: Isothermal; Col… (show more)umn class: Semi-stan

non-polar; Column type: Packed; Start T: 130 C; CAS no: 97870; Active p
Apiezon L; Data type: Kovats RI; Authors: Bogoslovsky, Yu. N.; Anvaer, B.
Vigdergauz, M. S., Chromatographic constants in gas chromatography (ir
Russian), Standards Publ. House, Moscow, 1978, 192.)NIST Spectranist ri

895 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column type: Packed; Start T: 120 C; CAS no: 97870; Active phase
Apiezon L; Substrate: Celite 545; Data type: Kovats RI; Authors: Bogoslov
N.; Anvaer, B. I.; Vigdergauz, M. S., Chromatographic constants in gas
chromatography (in Russian), Standards Publ. House, Moscow, 1978, 192
Spectranist ri

908 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column type: Packed; Start T: 160 C; CAS no: 97870; Active phase
Apiezon L; Substrate: Celite 545; Data type: Kovats RI; Authors: Bogoslov
N.; Anvaer, B. I.; Vigdergauz, M. S., Chromatographic constants in gas
chromatography (in Russian), Standards Publ. House, Moscow, 1978, 192
Spectranist ri

891 (Program type: Isothermal; Col... (show more)umn class: Semi-stand
polar; Column type: Packed; Start T: 70 C; CAS no: 97870; Active phase:
Squalane; Substrate: Chromosorb G; Data type: Kovats RI; Authors: Mira,
Sanchez, L. G., Polarity of the Gas Chromatographic Stationary Phases an
Retention Indices of Aliphatic Esters, Ketones and Alcohols, Anal. Chim. A
1970, 315-321.)NIST Spectranist ri

898 (Program type: Isothermal; Col... (show more)umn class: Semi-stand

polar; Column length: 2. 25 m; Column type: Packed; Start T: 190 C; CAS
97870; Active phase: Apiezon L; Substrate: Celite; Data type: Kovats RI; A
Wehrli, A.; Kovats, E., Gas-chromatographische Charakterisierung ograni
Verbindungen. Teil 3: Berechnung der Retentionsindices aliphatischer,
alicyclischer und aromatischer Verbindungen, Helv. Chim. Acta, 7, 1959,
2736.)NIST Spectranist ri

1149 (Program type: Ramp; Column cl… (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 2 K/min; Start T: 60 C; End T: 200 C; Start time: 10 min; CAS no: 97
Active phase: DB-Wax; Carrier gas: N2; Data type: Kovats RI; Authors: Ur
Shoji, A.; Hagi, Y.; Shibamoto, T., Volatile constituents of peel of quince fr
Cydonia oblonga Miller, J. Agric. Food Chem., 34(4), 1986, 593-596.)NIST
Spectranist ri

1145 (Program type: Isothermal; Col… (show more)umn class: Standard
Column length: 3 m; Column type: Packed; Start T: 100 C; CAS no: 97870
phase: Carbowax 20M; Substrate: Chromosorb WAW (60-80 mesh); Data
Kovats RI; Authors: Chastrette, M.; Heintz, M.; Druilhe, A.; Lefort, D., Ana
chromatographique d’esters aliphatiques satures. Relations retention-str
et prevision de la retention, Bull. Soc. Chim. Fr., , 1974, 1852-1856.)NIST
Spectranist ri

1197 (Program type: Isothermal; Col… (show more)umn class: Standard
Column length: 2 m; Column type: Packed; Start T: 100 C; CAS no: 97870
phase: Carbowax 20M; Substrate: Chromosorb W; Data type: Kovats RI; A
Zarazir, D.; Chovin, P.; Guiochon, G., Identification of hydroxylic compoun

their derivatives by gas chromatography, Chromatographia, 3, 1970, 180
195.)NIST Spectranist ri

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

934 (Program type: Ramp; Column cl... (show more)ass: Standard non-po
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 5 K/min; Start T: 30 C; End T: 210 C; CAS no: 97870; Active phase:
Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI;
Kumazawa, K.; Itobe, T.; Nishimura, O.; Hamaguchi, T., A new approach t
estimate the in-mouth release characteristics of odorants in chewing gur
Science and Technology Research, 14(3), 2008, 269-276.)NIST Spectrani

931 (Program type: Ramp; Column cl... (show more)ass: Standard non-po
Column type: Capillary; CAS no: 97870; Active phase: SE-30; Data type:
alkane RI; Authors: Liu, F.; Liang, Y.; Cao, C.; Zhou, N., QSPR study of GC
retention indices for saturated esters on seven stationary phases based
topological indices, Talanta, 72, 2007, 1307-1315.)NIST Spectranist ri

939 (Program type: Ramp; Column cl... (show more)ass: Standard non-po
Column diameter: 0. 28 mm; Column length: 50 m; Column type: Capilla
rate: 2 K/min; Start T: 80 C; End T: 200 C; CAS no: 97870; Active phase:
Data type: Normal alkane RI; Authors: Anker, L. S.; Jurs, P. C.; Edwards, P
Quantitative structure-retention relationship studies of odor-active alipha
compounds with oxygen-containing functional groups, Anal. Chem., 62, 1
2676-2684., Program type: Ramp; Column cl... (show more)ass: Standard
polar; Column type: Capillary; CAS no: 97870; Active phase: SE-30; Data
Normal alkane RI; Authors: Vinogradov, B. A., Production, composition, p

and application of essential oils, 2004.)NIST Spectranist ri

945 (Program type: Ramp; Column cl... (show more)ass: Standard non-po
Column type: Capillary; Heat rate: 2 K/min; Start T: 70 C; End T: 170 C; C
97870; Active phase: SE-30; Carrier gas: Helium; Data type: Normal alka
Authors: Alves, S.; Jennings, W. G., Volatile composition of certain Amazo
fruits, Food Chem., 4(2), 1979, 149-159.)NIST Spectranist ri

944 (Program type: Isothermal; Col... (show more)umn class: Standard n
Column type: Packed; Start T: 70 C; CAS no: 97870; Active phase: SE-30;
type: Normal alkane RI; Authors: Yabumoto, K.; Jennings, W. G.; Yamagu
Gas chromatographic retention as identification criteria, Anal. Biochem.,
1977, 244-251.)NIST Spectranist ri

911 (Program type: Ramp; Column cl... (show more)ass: Semi-standard n
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Heat rate: 4 K/min; Start T: 50 C; End T: 230 C; End time: 10 min; Start ti
min; CAS no: 97870; Active phase: HP-5 MS; Carrier gas: Helium; Phase
thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Forero, M. D.;
Quijano, C. E.; Pino, J. A., Volatile compounds of Chile pepper (Capsicum
L. var. glabriusculum) at two ripening stages, Flavour Fragr. J., 24, 2008,
30.)NIST Spectranist ri

1129 (Program type: Complex; Column... (show more)class: Standard po
Column diameter: 0. 20 mm; Column length: 50 m; Column type: Capilla
Description: 70 0C (1 min) ^ 3 0C/min -> 142 0C ^ 5 0C/min -> 225 0C (
CAS no: 97870; Active phase: FFAP; Carrier gas: Helium; Phase thickness

um; Data type: Normal alkane RI; Authors: Ortiz, A.; Echeverra, G.; Grael
Lara, I., Calcium dips enhance volatile emission of cold-stored “ Fuji Kiki-
apples, J. Agric. Food Chem., 57(11), 2009, 4931-4938.)NIST Spectranist

1149 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla
rate: 5 K/min; Start T: 30 C; End T: 210 C; CAS no: 97870; Active phase:
Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI;
Kumazawa, K.; Itobe, T.; Nishimura, O.; Hamaguchi, T., A new approach t
estimate the in-mouth release characteristics of odorants in chewing gur
Science and Technology Research, 14(3), 2008, 269-276.)NIST Spectrani

1139 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 2 mm; Column length: 80 m; Column type: Capillary
rate: 2 K/min; Start T: 70 C; End T: 170 C; CAS no: 97870; Active phase:
Carbowax 20M; Data type: Normal alkane RI; Authors: Anker, L. S.; Jurs,
Edwards, P. A., Quantitative structure-retention relationship studies of oc
active aliphatic compounds with oxygen-containing functional groups, An
Chem., 62, 1990, 2676-2684., Program type: Ramp; Column cl... (show m
Standard polar; Column type: Capillary; CAS no: 97870; Active phase: Ca
20M; Data type: Normal alkane RI; Authors: Vinogradov, B. A., Production
composition, properties and application of essential oils, 2004.)NIST Spec
ri

1159 (Program type: Ramp; Column cl... (show more)ass: Standard polar
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla
rate: 4 K/min; Start T: 60 C; End T: 220 C; End time: 10 min; Start time: 1

CAS no: 97870; Active phase: Innowax; Carrier gas: He; Data type: Norm
RI; Authors: Suleimenov, E. M.; Atazharova, G. A.; Demirchi, B.; Baser, K.
Adekenov, S. M., Essential oil composition of Artemisia Lercheana and A.
Sieversiana of Kazakhstan flora, in Recent problems of development of n
medicines of natural origin, Proceedings of symposium, St. Petersburg –
2003, 382-385.)NIST Spectranist ri

1147 (Program type: Isothermal; Col... (show more)umn class: Standard
Column type: Packed; Start T: 100 C; CAS no: 97870; Active phase: Carb
20M; Data type: Normal alkane RI; Authors: Yabumoto, K.; Jennings, W. G
Yamaguchi, M., Gas chromatographic retention as identification criteria,
Biochem., 78, 1977, 244-251.)NIST Spectranist ri

- **Retention Index (Linear):**

952 (Program type: Complex; Column... (show more)class: Standard non
Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capilla
Description: -20C (5min) => 10C/min => 100C => 4C/min => 200C =>
=> 280C; CAS no: 97870; Active phase: DB-1; Carrier gas: He; Phase thi
0. 25 um; Data type: Linear RI; Authors: Eri, S.; Khoo, B. K.; Lech, J.; Hart
G., Direct thermal desorption-gas chromatography and gas chromatogra
mass spectrometry profiling of hop (Humulus lupulus L.) essential oils in
of varietal characterization, J. Agric. Food Chem., 48, 2000, 1140-1149.)N
Spectranist ri

954 (Program type: Ramp; Column cl... (show more)ass: Semi-standard n
polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C
Heat rate: 20 K/min; Start T: 50 C; End T: 220 C; End time: 2 min; Start ti

min; CAS no: 97870; Active phase: SPB-5; Carrier gas: He; Phase thickne

um; Data type: Linear RI; Authors: Balbontin, C.; Gaete-Eastman, C.; Verg

Herrera, R.; Moya-Leon, M. A., Treatment with 1-MCP and the role of ethy

aroma development of mountain papaya fruit, Postharvest Biol. Technol.

2007, 67-77.)NIST Spectranist ri

955 (Program type: Ramp; Column cl… (show more)ass: Semi-standard n

polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C

Heat rate: 4 K/min; Start T: 60 C; End T: 250 C; End time: 20 min; Start ti

min; CAS no: 97870; Active phase: HP-5MS; Carrier gas: He; Phase thickn

25 um; Data type: Linear RI; Authors: Pino, J. A.; Mesa, J.; Munoz, Y.; Mart

Marbot, R., Volatile components from mango (Mangifera indica L.) cultiva

Agric. Food Chem., 53, 2005, 2213-2223.)NIST Spectranist ri

1154 (Program type: Complex; Column… (show more)class: Standard po

Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capilla

Description: 35C(8min) => 4C/min => 60C => 6C/min => 160C=> 20C

200C(1min); CAS no: 97870; Active phase: Supelcowax-10; Carrier gas: H

Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Bianchi, F.; Car

Mangia, A.; Musci, M., Retention indices in the analysis of food aroma vol

compounds in temperature-programmed gas chromatography: Database

creation and evaluation of precision and robustness, J. Sep. Sci., 39, 200

572.)NIST Spectranist ri

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

PhysChem Module

Density:	0. 9±0. 1 g/cm ^{3}
Boiling Point:	156. 3±8. 0 °C at 760 mmHg
Vapour Pressure:	2. 9±0. 3 mmHg at 25°C
Enthalpy of Vaporization:	39. 3±3. 0 kJ/mol
Flash Point:	46. 7±8. 3 °C
Index of Refraction:	1. 411
Molar Refractivity:	40. 8±0. 3 cm ^{3}
#H bond acceptors:	2
#H bond donors:	0
#Freely Rotating Bonds:	5
#Rule of 5 Violations:	0
ACD/LogP:	2. 65
ACD/LogD (pH 5. 5):	2. 42
ACD/BCF (pH 5. 5):	40. 51
ACD/KOC (pH 5. 5):	492. 37
ACD/LogD (pH 7. 4):	2. 42

ACD/BCF (pH 7. 4):	40. 51
ACD/KOC (pH 7. 4):	492. 37
Polar Surface Area:	26 Å ^{2}
Polarizability:	16. 2±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	26. 3±3. 0 dyne/cm
Molar Volume:	164. 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) = 2. 76Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 157. 09 (Adapted Stein & Brown method)Melting Pt (deg C): -43. 92 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 3. 18 (Mean VP of Antoine & Grain methods)MP (exp database): 8 at 25 deg C : 3. 709E-002 L/mol-secKb Half-Life at pH 8: 216. 263 days Kb Half-Life at pH 7: 5. 921 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 1. 421 (BCF = 26. 39)log Kow used: 2. 76 (estimated)Volatilization from Water: Henry LC: 0. 000974 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 1. 947 hoursHalf-Life from Model Lake : 121. 9 hours (5. 081 days)Removal In Wastewater Treatment: Total removal: 31. 55 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 3. 28 percentTotal to Air: 28. 18 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 9. 92 46. 7 1000 Water 25 208 1000 Soil 64. 9 416 1000 Sediment 0. 216 1. 87e+003 0 Persistence Time: 216 hr

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- 1-Click Scaffold Hop