

Benzenepropanoic
acid, 3,4-
bis[(trimethylsilyl)oxy]
-, trimethylsilyl ester
C₁₈H₃₄...



**ASSIGN
BUSTER**

Contents

- Retention Index (Linear):

Molecular
Formula $C_{18}H_{34}O_4Si_3$

Average mass 398. 717 Da

Density $1. 0 \pm 0. 1 \text{ g/cm}^3$

Boiling Point $373. 1 \pm 42. 0 \text{ }^\circ\text{C}$ at 760
mmHg

Flash Point $149. 1 \pm 23. 4 \text{ }^\circ\text{C}$

Molar
Refractivity $113. 8 \pm 0. 3 \text{ cm}^3$

Polarizability $45. 1 \pm 0. 5 \cdot 10^{-24} \text{ cm}^3$

Surface Tension $24. 6 \pm 3. 0 \text{ dyne/cm}$

Molar Volume $412. 2 \pm 3. 0 \text{ cm}^3$

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

- **Retention Index (Kovats):**

1886 (estimated with error: 89)NIST

Spectramainlib_292706, replib_16966

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

1935 (Program type: Ramp; Column cl... (show more)ass: Semi-standard

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

Heat rate: 4 K/min; Start T: 70 C; End T: 280 C; End time: 3 min; Start tim

min; CAS no: 27750670; Active phase: HP-5MS; Carrier gas: He; Phase th

0. 25 um; Data type: Normal alkane RI; Authors: Lee, B. Y.; Yanamandra,

Thurmon, T. F., Quantitative estimation of organic analytes with a capilla

column, Am. Clin. Lab., , 2002, 30-34.)NIST Spectranist ri

1923 (Program type: Ramp; Column cl... (show more)ass: Semi-standard

polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: C

Heat rate: 5 K/min; Start T: 70 C; End T: 280 C; Start time: 10 min; CAS n

27750670; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 52 um

type: Normal alkane RI; Authors: Richards, M.; Wong, Y. S.; Tan, W. C.; Ta

Ng, T. L., Profiling urinary organic acids for the diagnosis of inborn errors

metabolism by GC/MS, Bull. Sing. N. I. Chem., 20, 1992, 135-143.)NIST

Spectranist ri

- **Retention Index (Linear):**

1928 (Program type: Ramp; Column cl... (show more)ass: Standard non-p

Column diameter: 0. 15 mm; Column length: 25 m; Column type: Capilla

rate: 10 K/min; Start T: 90 C; End T: 270 C; End time: 7 min; Start time: 1

CAS no: 27750670; Active phase: CP Sil 5 CB; Phase thickness: 0.12 µm; Data type: Linear RI; Authors: Halket, J. N.; Przyborowska, A.; Stein, S. E.; Mallat, G.; Down, S.; Chalmers, R., Deconvolution gas chromatography / mass spectrometry of urinary organic acids - potential for pattern recognition and automated identification of metabolic disorders, Rapid Commun. Mass Spectrom. 13, 1999, 279-284.)NIST Spectranist ri

1907 (Program type: Ramp; Column classification: (show more) Standard non-polar; Column diameter: 0.53 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 70 C; End T: 290 C; CAS no: 27750670; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 1 µm; Data type: Linear RI; Authors: Halket, J. N.; Aramaki, S.; Blum-Hoffmann, E.; Nyhan, W. L.; Sweetman, L., Quantitative analysis for organic acids in biological samples: batch isolation followed by gas chromatographic-mass spectrometric analysis, Clin. Chem., 35(4), 1989, 595.)NIST Spectranist ri

1910 (Program type: Ramp; Column classification: (show more) Standard non-polar; Column diameter: 0.22 mm; Column length: 10 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 70 C; End T: 270 C; CAS no: 27750670; Active phase: CP Sil 5 CB; Carrier gas: He; Phase thickness: 0.17 µm; Data type: Linear RI; Authors: Lefevre, M. F.; Verhaeghe, B. J.; Declerck, D. H.; Van Bocxlaer, J. F.; De Leenheer, A. P.; De Sagher, R. M., Metabolic Profiling of Urinary Organic Acids by Single and Multicolumn Capillary Gas Chromatography, J. Chromatogr. Sci. 1989, 23-29.)NIST Spectranist ri

1908 (Program type: Ramp; Column classification: (show more) Standard non-polar; Column type: Capillary; Heat rate: 6 K/min; Start T: 60 C; End T: 280 C; E

5 min; Start time: 0.5 min; CAS no: 27750670; Active phase: CP Sil 5 CB
gas: N2; Data type: Linear RI; Authors: Wurth, C.; Kumps, A.; Mardens, Y.
organic acids: Retention indices on two capillary gas chromatography columns
Chromatogr., 491, 1989, 186-192.)NIST Spectranist ri

1906 (Program type: Ramp; Column classification: (show more)ass: Standard non-polar
Column type: Capillary; CAS no: 27750670; Active phase: DB-1; Carrier gas: N2
Data type: Linear RI; Authors: Tsai, M. Y.; Oliphant, C.; Josephson, M. W.,
Identification of Metabolites Diagnostic for Organic Acidurias by Simultaneous
Dual-Column Capillary Gas Chromatography, J. Chromatogr., 341, 1985,
10.)NIST Spectranist ri

1909 (Program type: Ramp; Column classification: (show more)ass: Standard non-polar
Column length: 1.8 m; Column type: Packed; Heat rate: 28 K/min; Start T: 100 C
End T: 290 C; Start time: 0.5 min; CAS no: 27750670; Active phase: OV-1
gas: N2; Substrate: 100-120 mesh; Data type: Linear RI; Authors: Tanaka,
Hine, D. G.; West-Dull, A.; Lynn, T. B., Gas-chromatographic method of analysis
for urinary organic acids. I. Retention indices of 155 metabolically important
compounds, Clin. Chem., 26(13), 1980, 1839-1846.)NIST Spectranist ri

1912 (Program type: Ramp; Column classification: (show more)ass: Standard non-polar
Column length: 2 m; Column type: Packed; Heat rate: 4 K/min; Start T: 80 C
End T: 240 C; CAS no: 27750670; Active phase: OV-1; Carrier gas: N2; Substrate:
Supelcoport; Data type: Linear RI; Authors: Mattsson, M.; Petersson, G.,
Reference GLC Data for the Analysis of Phenolic Compounds as Trimethylsilyl
Derivatives, J. Chromatogr. Sci., 15, 1977, 546-554., Program type: Ramp
Column classification: (show more)ass: Standard non-polar; Column length: 6 ft; Co

type: Packed; Heat rate: 10 K/min; Start T: 100 C; End T: 325 C; CAS no: 27750670; Active phase: OV-1; Carrier gas: He; Substrate: Chromosorb W (100 mesh); Data type: Linear RI; Authors: Butts, W. C., Two-Column Gas Chromatography of Trimethylsilyl Derivatives of Biochemically Significant Compounds, *Anal. Biochemistry*, 46, 1972, 187-199.)NIST Spectranist ri

1919 (Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 100 C; End T: 300 C; End time: 15 min; Start time: 4 min; CAS no: 27750670; Active phase: DB-5; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Ohie, T.; Fu, X.; Iga, M.; Kimura, M.; Yamaguchi, S., Automated gas chromatography-mass spectrometry with tert .-butyldimethylsilyl derivatives: use of the simplified sample preparations and the automated data system to screen for organic acidemias, *J. Chromatogr. B*, 746, 2000, 63-73., Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 100 C; End T: 290 C; End time: 10 min; Start time: 4 min; CAS no: 27750670; Active phase: DB-5; Carrier gas: He; Phase thickness: 1 um; Data type: Linear RI; Authors: Kimura, M.; Yamamoto, T.; Yamaguchi, S., Automated metabolic profiling and interpretation of GC/MS data for organic acidemia screening using a personal computer-based system, *Tohoku J. Exp. Med.*, 188, 1999, 317-324.)NIST Spectranist ri

1894 (Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0. 31 mm; Column length: 25 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 100 C; End T: 290 C; End time: 15 min; Start time: 4 min; CAS no: 27750670; Active phase: DB-5; Carrier gas: He; Phase thickness: 1 um; Data type: Linear RI; Authors: Kimura, M.; Yamamoto, T.; Yamaguchi, S., Automated metabolic profiling and interpretation of GC/MS data for organic acidemia screening using a personal computer-based system, *Tohoku J. Exp. Med.*, 188, 1999, 317-324.)NIST Spectranist ri

min; CAS no: 27750670; Active phase: HP-5; Carrier gas: He; Phase thickness: 0.52 um; Data type: Linear RI; Authors: Antoshechkin, A. G.; Golovkin, A. B.; Maximova, L. A.; Bakharev, V. A., Screening of amniotic fluid metabolites by gas chromatography-mass spectrometry, J. Chromatogr., 489, 1989, 353-358.)NIST Spectranist ri

1920 (Program type: Ramp; Column class: (show more)ass: Semi-standard non-polar; Column diameter: 0.32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 70 C; End T: 270 C; CAS no: 27750670; Active phase: SE-52; Carrier gas: He; Phase thickness: 0.52 um; Data type: Linear RI; Authors: Lefevre, M. F.; Verhaeghe, B. J.; Declerck, D. H.; Van Bocxlaer, J. F.; De Leenheer, A. P.; De Sagher, R. M., Metabolic Profiling of Urinary Organic Acids by Single and Multicolumn Capillary Gas Chromatography, J. Chromatogr. Sci., 1989, 23-29.)NIST Spectranist ri

1921 (Program type: Ramp; Column class: (show more)ass: Semi-standard non-polar; Column diameter: 0.31 mm; Column length: 25 m; Column type: Capillary; Heat rate: 5 K/min; Start T: 50 C; End T: 300 C; CAS no: 27750670; Active phase: Ultra-2; Carrier gas: He; Phase thickness: 0.52 um; Data type: Linear RI; Authors: Tuchman, M.; Bowers, L. D.; Fregien, K. D.; Crippin, P. J.; Krivit, W., Capillary Gas Chromatographic Separation of Urinary Organic Acids. Retention Indices and Identification of Urinary Acids on a 5% Phenylmethyl Silicone Capillary Column, J. Chromatogr. Sci., 22, 1984, 198-202.)NIST Spectranist ri

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

[https://assignbuster.com/benzenepropanoic-acid-4-bis\(trimethylsilyloxy\)-trimethylsilyl-ester-c18h34o4si3-structure/](https://assignbuster.com/benzenepropanoic-acid-4-bis(trimethylsilyloxy)-trimethylsilyl-ester-c18h34o4si3-structure/)

Density:	1.0 ± 0.1 g/cm ³
Boiling Point:	373.1 ± 42.0 °C at 760 mmHg
Vapour Pressure:	0.0 ± 0.8 mmHg at 25°C
Enthalpy of Vaporization:	62.0 ± 3.0 kJ/mol
Flash Point:	149.1 ± 23.4 °C
Index of Refraction:	1.464
Molar Refractivity:	113.8 ± 0.3 cm ³
#H bond acceptors:	4
#H bond donors:	0
#Freely Rotating Bonds:	9
#Rule of 5 Violations:	0
ACD/LogP:	2.22
ACD/LogD (pH 5.5):	3.06
ACD/BCF (pH 5.5):	124.09
ACD/KOC (pH 5.5):	1097.23
ACD/LogD (pH 7.4):	3.06

ACD/BCF (pH 7.4):	124.09
ACD/KOC (pH 7.4):	1097.23
Polar Surface Area:	45 Å ²
Polarizability:	45.1 ± 0.5 × 10 ⁻²⁴ cm ³
Surface Tension:	24.6 ± 3.0 dyne/cm
Molar Volume:	412.2 ± 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) = 7.14
Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.42):
Boiling Pt (deg C): 356.22 (Adapted Stein & Brown method) Melting Pt (deg C): 98.83 (Mean or Weighted MP)
VP (mm Hg, 25 deg C): 1.8E-005 (Modified Grain method) Subcooled liquid VP: 9.39E-005 mm Hg (25 deg C, Mod-Grain method)
Water Solubility Estimate from Log Kow (WSKOW v1.41): Water Solubility at 25 deg C (mg/L): 0.002502
log Kow used: 7.14 (estimated) no-melting pt equation used
Water Sol Estimate from Fragments: Wat Sol (v1.01 est) = 32.951 mg/L
ECOSAR Class Program (ECOSAR v0.99h): Class(es) found: Esters
Silanes (alkoxy) Henry's Law Constant (25 deg C) [HENRYWIN v3.10]: Bond Method: 6.09E-004 atm-m³/mole
Group Method: Incomplete Henry's LC [VP/WSol estimate using EPI values]: 3.774E-003 atm-m³/mole
Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]: Log Kow used: 7.14 (KowWin est)
Log Kaw used: -1.604 (HenryWin est) Log Koa (KOAWIN v1.10 estimate): 8.744
Log Koa (experimental database): None
Probability of Rapid Biodegradation (BIOWIN v4.10): Biowin1 (Linear Model): 0.6124
Biowin2 (Non-Linear Model): 0.1114
Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2.2432 (months)
Biowin4 (Primary Survey Model): 3.2039 (weeks)
MITI Biodegradation Probability: Biowin5 (MITI Linear Model): -0.5439
Biowin6 (MITI Non-Linear Model): 0.0002
Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0.5494
Ready Biodegradability Prediction: NO
Hydrocarbon Biodegradation (BioHCwin v1.01): Structure incompatible with current estimation method!
Sorption to aerosols (25 Dec C) [AEROWIN v1.00]: Vapor pressure (liquid/subcooled): 0.0125 Pa (9.39E-005 mm Hg)
Log Koa (Koawin est): 8.744
Kp (particle/gas partition coef. (m³/ug)): Mackay model: 0.00024
Octanol/air (Koa) model: 0.000136
Fraction sorbed to

[https://assignbuster.com/benzenepropanoic-acid-4-bis\(trimethylsilyloxy\)-trimethylsilyl-ester-c18h34o4si3-structure/](https://assignbuster.com/benzenepropanoic-acid-4-bis(trimethylsilyloxy)-trimethylsilyl-ester-c18h34o4si3-structure/)

airborne particulates (phi): Junge-Pankow model : 0. 00858 Mackay model : 0. 0188 Octanol/air (Koa) model: 0. 0108 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 33. 2062 E-12 cm³/molecule-sec Half-Life = 0. 322 Days (12-hr day; 1. 5E6 OH/cm³) Half-Life = 3. 865 Hrs Ozone Reaction: No Ozone Reaction Estimation Fraction sorbed to airborne particulates (phi): 0. 0137 (Junge, Mackay) Note: the sorbed fraction may be resistant to atmospheric oxidation Soil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 2. 237E+005 Log Koc: 5. 350 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 = 4. 621 (BCF = 4. 182e+004) log Kow used: 7. 14 (estimated) Volatilization from Water: Henry LC: 0. 000609 atm-m³/mole (estimated by Bond SAR Method) Half-Life from Model River: 3. 957 hours Half-Life from Model Lake : 210. 6 hours (8. 775 days) Removal In Wastewater Treatment: Total removal: 93. 90 percent Total biodegradation: 0. 78 percent Total sludge adsorption: 93. 09 percent Total to Air: 0. 04 percent (using 10000 hr Bio P, A, S) Level III Fugacity Model: Mass Amount Half-Life Emissions (percent) (hr) (kg/hr) Air 0. 077 7. 73 1000 Water 1. 51 1. 44e+003 1000 Soil 31 2. 88e+003 1000 Sediment 67. 4 1. 3e+004 0 Persistence Time: 4. 48e+003 hr

Click to predict properties on the Chemicalize site