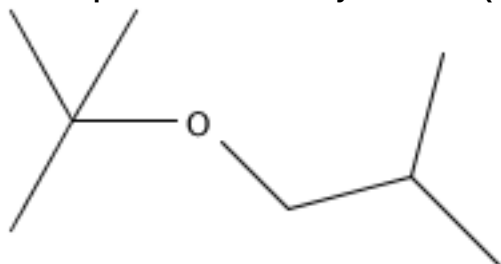


Task History

Task Began October 06, 2016 09:59 AM

Explore substances by EXACT ID(1)

*Answer Type:**Substances**Result Count:*

4

Detailed display

From ID:

1

Type:

33021-02-2

CAS Registry Number: 33021-02-2

 $C_8H_{18}O$

Propane, 1-(1,1-dimethylethoxy)-2-methyl-

Molecular Weight

130.23

Melting Point (Experimental)

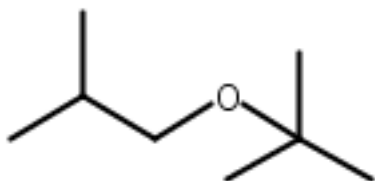
Value: -111.008--110.829 °C

Boiling Point (Experimental)

Value: 113.18 °C

Density (Experimental)Value: 0.7516 g/cm³ | Condition: Temp: 20 °C

Other Names: Ether, *tert*-butyl isobutyl (6CI); 1-(1,1-Dimethylethoxy)-2-methylpropane; 1-*tert*-Butoxy-2-methylpropane; Isobutyl *tert*-butyl ether; *tert*-Butyl isobutyl ether



~80 References

~9 Commercial Sources

Experimental Properties: Density Interface Optical and Scattering Spectra Thermal

Density Properties	Value	Condition	Note
Density	0.755 g/cm ³	Temp: 20 °C	(5)CAS
Density	0.7516 g/cm ³	Temp: 20 °C	(1)CAS
Density	See full text		(7)CAS
Density	See full text		(8)CAS
Interface Properties	Value	Condition	Note
Vapor Pressure/Volatility	See full text		(7)CAS
Vapor Pressure/Volatility	See full text		(9)CAS
Vapor Pressure/Volatility	See full text		(8)CAS
Optical and Scattering Properties	Value	Condition	Note
Refractive Index	1.393	Wavlen: 589.3 nm; Temp: 20 °C	(5)CAS
Refractive Index	1.3912	Wavlen: 589.3 nm	(6)CAS
Thermal Properties	Value	Condition	Note
Boiling Point	114 °C		(1)CAS
Boiling Point	114 °C	Press: 760 Torr	(2)IC
Boiling Point	113.18 °C		(3)CAS
Boiling Point	111.5 °C		(4)CAS
Boiling Point	111-112 °C		(5)CAS
Boiling Point	110-111 °C		(6)CAS
Boiling Point	See full text		(7)CAS
Boiling Point	See full text		(8)CAS
Boiling Point	See full text		(9)CAS
Enthalpy	See full text		(7)CAS
Enthalpy	See full text		(10)CAS
Enthalpy	See full text		(8)CAS
Enthalpy	See full text		(11)CAS
Enthalpy	See full text		(9)CAS
Entropy	See full text		(10)CAS
Formation Enthalpy	See full text		(10)CAS
Fusion Enthalpy	See full text		(10)CAS
Fusion Entropy	See full text		(10)CAS
Gibbs Free Energy	See full text		(10)CAS

Glass Transition Temperature	-159.1 °C	(10)CAS	
Heat Capacity	See full text	(10)CAS	
Heat Capacity	See full text	(11)CAS	
Melting Point	-111.008--110.829 °C	(10)CAS	
Melting Point	-132 °C	(2)IC	
Melting Point	See full text	(7)CAS	
Triple Point	See full text	(10)CAS	
Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See full text		(4)CAS
Mass Spectrum	See spectrum		(12)WSS
Proton NMR Spectrum	See full text		(4)CAS

- (1) Evans, T. W.; Industrial and Engineering Chemistry 1936, V28, P1186-8 CAPLUS
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- (3) Evans, Theodore; US 2010356 1935 CAPLUS
- (4) Grabovskiy, S. A.; Russian Chemical Bulletin 2005, V54(10), P2384-2393 CAPLUS
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- (7) Krasnykh, E. L.; Neftekhimiya 2005, V45(2), P111-114 CAPLUS
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- (9) Efimova, A. A.; Journal of Chemical Thermodynamics 2006, V39(1), P142-147 CAPLUS
- (10) Druzhinina, A. I.; Journal of Chemical Thermodynamics 2006, V38(1), P10-19 CAPLUS
- (11) Verevkin, Sergey P.; Journal of Chemical and Engineering Data 2003, V48(3), P591-599 CAPLUS
- (12) WSS: Spectral data were obtained from Wiley Subscription Services, Inc. (US)

Predicted Properties: Biological Chemical Density Lipinski Spectra Structure Related Thermal

Biological Properties	Value	Condition	Note
Bioconcentration Factor	62.8	pH 1 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 2 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 3 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 4 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 5 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 6 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 7 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 8 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 9 Temp: 25 °C	(13)
Bioconcentration Factor	62.8	pH 10 Temp: 25 °C	(13)
Chemical Properties	Value	Condition	Note
Koc	674	pH 1 Temp: 25 °C	(13)
Koc	674	pH 2 Temp: 25 °C	(13)
Koc	674	pH 3 Temp: 25 °C	(13)
Koc	674	pH 4 Temp: 25 °C	(13)
Koc	674	pH 5 Temp: 25 °C	(13)
Koc	674	pH 6 Temp: 25 °C	(13)
Koc	674	pH 7 Temp: 25 °C	(13)
Koc	674	pH 8 Temp: 25 °C	(13)
Koc	674	pH 9 Temp: 25 °C	(13)
Koc	674	pH 10 Temp: 25 °C	(13)
logD	2.67	pH 1 Temp: 25 °C	(13)
logD	2.67	pH 2 Temp: 25 °C	(13)
logD	2.67	pH 3 Temp: 25 °C	(13)
logD	2.67	pH 4 Temp: 25 °C	(13)

logD	2.67	pH 5 Temp: 25 °C	(13)
logD	2.67	pH 6 Temp: 25 °C	(13)
logD	2.67	pH 7 Temp: 25 °C	(13)
logD	2.67	pH 8 Temp: 25 °C	(13)
logD	2.67	pH 9 Temp: 25 °C	(13)
logD	2.67	pH 10 Temp: 25 °C	(13)
logP	2.668±0.228	Temp: 25 °C	(13)
Mass Intrinsic Solubility	Slightly Soluble (3.0 g/L)	Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 1 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 2 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 3 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 4 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 5 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 6 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 7 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 8 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 9 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	pH 10 Temp: 25 °C	(13)
Mass Solubility	Slightly Soluble (3.0 g/L)	Unbuffered Water pH 7.00 Temp: 25 °C	(13)
Molar Intrinsic Solubility	Slightly Soluble (0.023 mol/L)	Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 1 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 2 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 3 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 4 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 5 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 6 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 7 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 8 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 9 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	pH 10 Temp: 25 °C	(13)
Molar Solubility	Slightly Soluble (0.023 mol/L)	Unbuffered Water pH 7.00 Temp: 25 °C	(13)
Molecular Weight	130.23		(13)
Vapor Pressure	21.2 Torr	Temp: 25 °C	(13)
Density Properties	Value	Condition	Note
Density	0.778±0.06 g/cm3	Temp: 20 °C Press: 760 Torr	(13)
Molar Volume	167.3±3.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(13)
Lipinski Properties	Value	Condition	Note
Freely Rotatable Bonds	3		(13)
H Acceptors	1		(13)
H Donors	0		(13)
H Donor/Acceptor Sum	1		(13)
logP	2.668±0.228	Temp: 25 °C	(13)
Molecular Weight	130.23		(13)
Structure Related Properties	Value	Condition	Note
Polar Surface Area	9.23 A2		(13)
Thermal Properties	Value	Condition	Note
Boiling Point	117.0±8.0 °C	Press: 760 Torr	(13)
Enthalpy of Vaporization	34.06±3.0 kJ/mol	Press: 760 Torr	(13)
Flash Point	13.7±10.2 °C		(13)
Spectra Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(14)
Proton NMR Spectrum	See spectrum		(14)

(13) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs)

(14) Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V11.01 (© 1994-2016 ACD/Labs)

REGULATORY INFORMATION :**Regulatory Synonyms**

1-(1,1-dimethylethoxy)-2-methylpropane (English, French) (REACH, EINECS)

1-(1,1-Dimethylethoxy)-2-methylpropan (German) (EINECS)

1-(1,1-dimetiletoxi)-2-metilpropano (Spanish) (EINECS)

1-tert-Butoxy-2-methylpropane

Ether, tert-butyl isobutyl

Isobutyl tert-butyl ether

Propane, 1-(1,1-dimethylethoxy)-2-methyl-

tert-Butyl isobutyl ether

Regulatory Overview by Country**Confidentiality Status**

Public

European Union**EU Customs Code CN:**

29091990

Inventory Status

On REACH

REACH: List of Registered Substances, 2015

On EINECS

Annex to Official Journal of the European Communities, 15 June 1990

Regulatory List Number

EC No.: 251-347-1

EINECS No.: 251-347-1

International and other lists**Harmonized Tariff Code**

290919

Regulatory Inventories**File Segment**

EEC: EINECS

EU: REACH

Harmonized Tariff Code: HTC

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study		✓		
Biological Study		✓		
Formation, Nonpreparative		✓		

Occurrence		✓
Preparation	✓	✓
Process	✓	✓
Properties		✓
Reactant or Reagent	✓	✓
Uses		✓

Document Type(s): Journal, Patent

Source of Registration: CA