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

Other names:	1-(1,1-dimethylethoxy)-2-methylpropane 1-isobutoxy-1,1-dimethylethane 1-tert-Butoxy-2-methylpropane 2,2,5-trimethyl-3-oxahexane 2-methylpropyl 1,1-dimethylethyl ether Isobutyl tert-butyl ether ethane, 1-isobutoxy-1,1-dimethyl- ether, isobutyl tert-butyl ether, tert-butyl isobutyl tert-Butyl Isobutyl ether
Inchi:	InChI=1S/C8H18O/c1-7(2)6-9-8(3,4)5/h7H,6H2,1-5H3
InchiKey:	UPOMCDPCTBJJDA-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CC(C)COC(C)(C)C
Mol. weight [g/mol]:	130.23
CAS:	33021-02-2

Physical Properties

Property code	Value	Unit	Source
chl	-5311.50 ± 1.20	kJ/mol	NIST Webbook
chl	-5311.50 ± 2.00	kJ/mol	NIST Webbook
gf	-88.12	kJ/mol	Joback Method
hf	-368.20 ± 2.00	kJ/mol	NIST Webbook
hf	-369.00 ± 1.60	kJ/mol	NIST Webbook
hfl	-409.10 ± 1.60	kJ/mol	NIST Webbook
hfl	-409.10 ± 2.00	kJ/mol	NIST Webbook
hfus	8.65	kJ/mol	The low-temperature heat capacity and ideal gas thermodynamic properties of isobutyl tert-butyl ether
hvap	40.10 ± 0.10	kJ/mol	NIST Webbook
hvap	40.90 ± 0.30	kJ/mol	NIST Webbook
hvap	41.20 ± 0.30	kJ/mol	NIST Webbook
hvap	40.12 ± 0.13	kJ/mol	NIST Webbook
hvap	39.12	kJ/mol	NIST Webbook
hvap	39.20 ± 0.30	kJ/mol	NIST Webbook
hvap	39.10 ± 0.50	kJ/mol	NIST Webbook
hvap	40.94 ± 0.30	kJ/mol	NIST Webbook

log10ws	-2.13		Crippen Method
logp	2.458		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	763.00		NIST Webbook
rinpol	748.80		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	750.20		NIST Webbook
rinpol	750.20		NIST Webbook
tb	385.20	K	NIST Webbook
tc	579.71	K	Joback Method
tf	189.57	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.44	J/mol×K	430.94	Joback Method
cpg	287.38	J/mol×K	460.70	Joback Method
cpg	300.73	J/mol×K	490.45	Joback Method
cpg	313.49	J/mol×K	520.20	Joback Method
cpg	325.69	J/mol×K	549.95	Joback Method
cpg	337.34	J/mol×K	579.71	Joback Method
cpg	258.89	J/mol×K	401.19	Joback Method
dvisc	0.0040597	Pa×s	224.84	Joback Method
dvisc	0.0002319	Pa×s	401.19	Joback Method
dvisc	0.0016788	Pa×s	260.11	Joback Method
dvisc	0.0008572	Pa×s	295.38	Joback Method
dvisc	0.0005052	Pa×s	330.65	Joback Method
dvisc	0.0003297	Pa×s	365.92	Joback Method
dvisc	0.0136359	Pa×s	189.57	Joback Method
hfust	8.65	kJ/mol	162.30	NIST Webbook
hvapt	33.11	kJ/mol	385.20	NIST Webbook
pvap	1.40	kPa	284.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	97.44	kPa	384.69	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	99.60	kPa	385.45	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	0.68	kPa	273.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.75	kPa	275.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.80	kPa	276.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.90	kPa	278.50	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.94	kPa	278.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.98	kPa	280.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	1.21	kPa	282.50	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	1.36	kPa	283.50	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	95.31	kPa	383.92	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether	
pvap	1.66	kPa	287.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	1.77	kPa	288.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	2.00	kPa	290.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	2.35	kPa	293.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	2.44	kPa	293.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	

pvap	2.69	kPa	295.60	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	3.19	kPa	298.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	3.15	kPa	298.70	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	3.72	kPa	301.80	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	4.03	kPa	303.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	4.45	kPa	304.80	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	5.22	kPa	308.40	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers	
pvap	93.18	kPa	383.13	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether	

pvap	81.57	kPa	378.59	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	67.49	kPa	372.35	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	56.12	kPa	366.48	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	45.83	kPa	360.31	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	37.26	kPa	354.26	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	30.91	kPa	349.00	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	25.07	kPa	343.33	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether

pvap	20.88	kPa	338.55	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	13.43	kPa	327.65	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	10.80	kPa	322.60	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	8.43	kPa	317.06	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	6.23	kPa	310.61	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether
pvap	16.83	kPa	333.13	The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44611e+01

Coeff. B	-3.54707e+03
Coeff. C	-5.37400e+01
Temperature range (K), min.	304.00
Temperature range (K), max.	441.41

Sources

The low-temperature heat capacity and ideal gas thermodynamic properties of isobutyl tert-butyl ether:	https://www.doi.org/10.1016/j.jct.2005.02.003
The thermodynamics of vaporization of ethyl tert-butyl ether, isobutyl tert-butyl ether, and di-isopropyl ether:	https://www.doi.org/10.1016/j.jct.2006.05.007
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers:	https://www.doi.org/10.1021/je0255980
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33021022&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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