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

Other names:	(i-C3H7)O(t-C4H9)
	1,1-dimethyl-1-isopropoxyethane
	1-methylethyl 1,1-dimethylethyl ether
	2,4,4-trimethyl-3-oxapentane
	2-Methyl-2-(1-methylethoxy)propane
	2-isopropoxy-2-methylpropane
	Ether, tert-butyl isopropyl
	ISOPROPYL-TERT-BUTYL ETHER
	Isopropyl tert-butyl ether
	ethane, 1,1-dimethyl-1-isopropoxy-
	ether, 1-methylethyl, 1,1-dimethylethyl
	ether, isopropyl tert-butyl
	tert-Butyl isopropyl ether
Inchi:	InChI=1S/C7H16O/c1-6(2)8-7(3,4)5/h6H,1-5H3
InchiKey:	HNFSPSWQNZVCTB-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CC(C)OC(C)(C)C
Mol. weight [g/mol]:	116.20
CAS:	17348-59-3

Physical Properties

Property code	Value	Unit	Source
affp	870.70	kJ/mol	NIST Webbook
basg	841.50	kJ/mol	NIST Webbook
chl	-4648.30 ± 2.80	kJ/mol	NIST Webbook
gf	-96.54	kJ/mol	Joback Method
hf	-358.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-393.00 ± 3.00	kJ/mol	NIST Webbook
hfus	4.14	kJ/mol	Joback Method
hvap	34.40 ± 0.60	kJ/mol	NIST Webbook
hvap	34.67	kJ/mol	NIST Webbook
hvap	34.50 ± 0.20	kJ/mol	NIST Webbook
hvap	36.20	kJ/mol	NIST Webbook
hvap	35.10	kJ/mol	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.210		Crippen Method

mcvol	115.360	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	643.50		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	631.00		NIST Webbook
rinpol	644.60		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	665.00		NIST Webbook
rinpol	644.60		NIST Webbook
ripol	720.00		NIST Webbook
ripol	724.00		NIST Webbook
ripol	724.00		NIST Webbook
tb	360.80 ± 0.40	K	NIST Webbook
tb	360.80 ± 0.50	K	NIST Webbook
tb	360.80	K	NIST Webbook
tb	360.70	K	NIST Webbook
tc	557.69	K	Joback Method
tf	185.08 ± 0.20	K	NIST Webbook
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.39	J/mol×K	378.31	Joback Method
cpg	232.76	J/mol×K	408.21	Joback Method
cpg	245.58	J/mol×K	438.10	Joback Method
cpg	257.86	J/mol×K	468.00	Joback Method
cpg	269.60	J/mol×K	497.90	Joback Method
cpg	280.83	J/mol×K	527.80	Joback Method
cpg	291.56	J/mol×K	557.69	Joback Method
dvisc	0.0042527	Pa×s	211.64	Joback Method
dvisc	0.0142654	Pa×s	178.30	Joback Method
dvisc	0.0017624	Pa×s	244.97	Joback Method
dvisc	0.0009019	Pa×s	278.31	Joback Method
dvisc	0.0005327	Pa×s	311.64	Joback Method
dvisc	0.0003483	Pa×s	344.98	Joback Method
dvisc	0.0002455	Pa×s	378.31	Joback Method
hfust	8.46	kJ/mol	184.80	NIST Webbook
hvapt	30.50	kJ/mol	360.70	NIST Webbook
hvapt	34.00	kJ/mol	333.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.97222e+01
Coeff. B	-7.49443e+03
Coeff. C	-1.28665e+01
Coeff. D	1.10706e-05
Temperature range (K), min.	306.15
Temperature range (K), max.	361.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1019.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17348593&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1019
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid liquid equilibria for binary systems of tert-amyl ethyl ether (TAEE), isopropyl tert-butyl ether (IPTBE) and di-sec-butyl ether (DSBE) with water and for ternary systems with methanol or ethanol:	https://www.doi.org/10.1016/j.fluid.2007.04.018
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume