2-Propanol, 1-(1,1-dimethylethoxy)-

Other names:	1-(1,1-dimethylethoxy)-2-propanol
	1-tert-butoxy-2-propanol
	monopeopyleenglycol
	propylene glycol mono-tert-butyl ether
Inchi:	InChI=1S/C7H16O2/c1-6(8)5-9-7(2,3)4/h6,8H,5H2,1-4H3
InchiKey:	GQCZPFJGIXHZMB-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CC(O)COC(C)(C)C
Mol. weight [g/mol]:	132.20
CAS:	57018-52-7

Physical Properties

Property code	Value	Unit	Source
gf	-233.36	kJ/mol	Joback Method
hf	-486.29	kJ/mol	Joback Method
hfus	8.22	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.182		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	2720.00	kPa	Critical Point and Vapor Pressure Measurements for Seven Compounds by a Low Residence Time Flow Method
rinpol	861.60		NIST Webbook
rinpol	862.00		NIST Webbook
tb	470.49	K	Joback Method
tc	643.77	K	Joback Method
tf	239.12	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	274.42	J/mol×K	470.49	Joback Method
cpg	286.06	J/mol×K	499.37	Joback Method
cpg	297.20	J/mol×K	528.25	Joback Method
cpg	307.84	J/mol×K	557.13	Joback Method
cpg	318.00	J/mol×K	586.01	Joback Method
cpg	327.70	J/mol×K	614.89	Joback Method
cpg	336.95	J/mol×K	643.77	Joback Method
dvisc	0.0888370	Pa×s	239.12	Joback Method
dvisc	0.0147686	Pa×s	277.68	Joback Method
dvisc	0.0038030	Pa×s	316.24	Joback Method
dvisc	0.0013152	Pa×s	354.81	Joback Method
dvisc	0.0005601	Pa×s	393.37	Joback Method
dvisc	0.0002778	Pa×s	431.93	Joback Method
dvisc	0.0001546	Pa×s	470.49	Joback Method
hvapt	45.40	kJ/mol	383.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32063e+01
Coeff. B	-3.39378e+03
Coeff. C	-5.71180e+01
Temperature range (K), min.	319.82
Temperature range (K), max.	486.99

Sources

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
Critical Point and Vapor Pressure Measurements for Seven Compounds by a Low Residence Time Flow Method:	https://www.doi.org/10.1021/je060088h
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57018527&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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