1,2-Propanediol, 2-methyl-

Other names: 2-Methyl-1,2-propanediol
2-methylpropane-1,2-diol
Inchi: InChI=1S/C4H10O2/c1-4(2,6)3-5/h5-6H,3H2,1-2H3
InchiKey: BTVWZWFKMIUSGS-UHFFFAOYSA-N
Formula: C4H10O2
SMILES: CC(C)(O)CO
Mol. weight [g/mol]: 90.12
CAS: 558-43-0

Physical Properties

Property code	Value	Unit	Source
chl	-2464.00	kJ/mol	NIST Webbook
gf	-288.00	kJ/mol	Joback Method
hf	-439.10	kJ/mol	Joback Method
hfl	-540.00	kJ/mol	NIST Webbook
hfus	6.88	kJ/mol	Joback Method
hvap	56.56	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	-0.250		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	5109.34	kPa	Joback Method
rinpol	816.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	718.00		NIST Webbook
tb	450.65 ± 2.00	K	NIST Webbook
tb	450.15 ± 3.00	K	NIST Webbook
tb	451.15 ± 2.00	K	NIST Webbook
tc	639.52	K	Joback Method
tf	258.90	K	Joback Method
vc	0.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.47	J/mol×K	472.05	Joback Method
cpg	208.41	J/mol×K	611.61	Joback Method
cpg	202.69	J/mol×K	583.70	Joback Method
cpg	196.65	J/mol×K	555.79	Joback Method
cpg	190.28	J/mol×K	527.87	Joback Method
cpg	183.56	J/mol×K	499.96	Joback Method
cpg	213.84	J/mol×K	639.52	Joback Method
dvisc	0.0001372	Pa×s	472.05	Joback Method
dvisc	0.0002913	Pa×s	436.52	Joback Method
dvisc	0.0007066	Pa×s	401.00	Joback Method
dvisc	0.0020364	Pa×s	365.47	Joback Method
dvisc	0.0073717	Pa×s	329.95	Joback Method
dvisc	0.0363990	Pa×s	294.42	Joback Method
dvisc	0.2785684	Pa×s	258.90	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64216e+01
Coeff. B	-4.53931e+03
Coeff. C	-6.65700e+01
Temperature range (K), min.	347.92
Temperature range (K), max.	475.14

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C558430&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvap:	Enthalpy of vaporization at standard conditions
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