1,3-Propanediol, 2-(hydroxymethyl)-

Other names:	Propane, 1,3-dihydroxy-2-hydroxymethyl- 2-(hydroxymethyl)propane-1,3-diol
Inchi:	InChI=1S/C4H10O3/c5-1-4(2-6)3-7/h4-7H,1-3H2
InchiKey:	SFRDXVJWXWOTEW-UHFFFAOYSA-N
Formula:	C4H10O3
SMILES:	OCC(CO)CO
Mol. weight [g/mol]:	106.12
CAS:	4704-94-3

Physical Properties

Property code	Value	Unit	Source
gf	-430.10	kJ/mol	Joback Method
hf	-587.86	kJ/mol	Joback Method
hfus	14.86	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	0.95		Crippen Method
logp	-1.420		Crippen Method
mcvol	84.830	ml/mol	McGowan Method
pc	5756.64	kPa	Joback Method
tb	567.02	K	Joback Method
tc	725.28	K	Joback Method
tf	302.30	K	Joback Method
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.49	J/mol×K	567.02	Joback Method
cpg	217.38	J/mol×K	593.40	Joback Method
cpg	223.03	J/mol×K	619.77	Joback Method
cpg	228.44	J/mol×K	646.15	Joback Method
cpg	233.64	J/mol×K	672.52	Joback Method
cpg	238.61	J/mol×K	698.90	Joback Method
cpg	243.37	J/mol×K	725.28	Joback Method

dvisc	0.1910150	Pa×s	302.30	Joback Method
dvisc	0.0160153	Pa×s	346.42	Joback Method
dvisc	0.0023509	Pa×s	390.54	Joback Method
dvisc	0.0005095	Pa×s	434.66	Joback Method
dvisc	0.0001463	Pa×s	478.78	Joback Method
dvisc	0.0000519	Pa×s	522.90	Joback Method
dvisc	0.0000216	Pa×s	567.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4704943&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume