R-(-)-1,2-propanediol

Other names: 1,2-Propanediol, (R)-
PROPANE-1,2-DIOL,(R)-(-)-
(R)-Propylene glycol
(R)-1,2-propanediol (propylene glycol)
Inchi: InChI=1S/C3H8O2/c1-3(5)2-4/h3-5H,2H2,1H3/t3-/m1/s1
InchiKey: DNIAPMSPPWPWGF-GSVOUGTGSA-N
Formula: C3H8O2
SMILES: CC(O)CO
Mol. weight [g/mol]: 76.09
CAS: 4254-14-2

Physical Properties

Property code	Value	Unit	Source
gf	-301.70	kJ/mol	Joback Method
hf	-414.99	kJ/mol	Joback Method
hfus	8.18	kJ/mol	Joback Method
hvap	55.24	kJ/mol	Joback Method
log10ws	0.28		Crippen Method
logp	-0.640		Crippen Method
mcvol	64.870	ml/mol	McGowan Method
pc	5791.74	kPa	Joback Method
tb	461.15 ± 2.00	K	NIST Webbook
tc	614.38	K	Joback Method
tf	230.21	K	Joback Method
vc	0.235	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.47	J/mol×K	451.96	Joback Method
cpg	140.93	J/mol×K	479.03	Joback Method
cpg	146.19	J/mol×K	506.10	Joback Method
cpg	151.24	J/mol×K	533.17	Joback Method
cpg	156.10	J/mol×K	560.24	Joback Method

cpg	160.76	J/mol×K	587.31	Joback Method
cpg	165.24	J/mol×K	614.38	Joback Method
dvisc	0.9647802	Pa×s	230.21	Joback Method
dvisc	0.0836198	Pa×s	267.17	Joback Method
dvisc	0.0131321	Pa×s	304.13	Joback Method
dvisc	0.0030803	Pa×s	341.08	Joback Method
dvisc	0.0009593	Pa×s	378.04	Joback Method
dvisc	0.0003678	Pa×s	415.00	Joback Method
dvisc	0.0001649	Pa×s	451.96	Joback Method
hfust	8.40	kJ/mol	240.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4254142&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
hfust: Enthalpy of fusion at a given temperature
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

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