(2R,4R)-(-)-Pentanediol

Other names: (2S,4S)-pentane-2,4-diol
(S,S)-2,4-pentanediol
[S-(R*,R*)]-2,4-pentanediol
Inchi: InChI=1S/C5H12O2/c1-4(6)3-5(2)7/h4-7H,3H2,1-2H3/t4-,5-/m0/s1
InchiKey: GTCCGKPBSJZVRZ-WHFBIAKZSA-N
Formula: C5H12O2
SMILES: CC(O)CC(C)O
Mol. weight [g/mol]: 104.15
CAS: 42075-32-1

Physical Properties

Property code	Value	Unit	Source
gf	-287.30	kJ/mol	Joback Method
hf	-461.55	kJ/mol	Joback Method
hfus	9.84	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.138		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	497.28	K	Joback Method
tc	661.20	K	Joback Method
tf	237.75	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.59	J/mol×K	497.28	Joback Method
cpg	249.98	J/mol×K	633.88	Joback Method
cpg	243.30	J/mol×K	606.56	Joback Method
cpg	236.33	J/mol×K	579.24	Joback Method
cpg	229.06	J/mol×K	551.92	Joback Method
cpg	221.48	J/mol×K	524.60	Joback Method

cpg	256.38	J/mol×K	661.20	Joback Method
dvisc	0.0000920	Pa×s	497.28	Joback Method
dvisc	0.0002095	Pa×s	454.02	Joback Method
dvisc	0.0005673	Pa×s	410.77	Joback Method
dvisc	0.0019427	Pa×s	367.51	Joback Method
dvisc	0.0092386	Pa×s	324.26	Joback Method
dvisc	0.0710068	Pa×s	281.00	Joback Method
dvisc	1.1462269	Pa×s	237.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	2.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42075321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpic Pairwise Interactions of Isomers of 2,4-pentanediol and 2,5-hexanediol in Dimethylsulfoxide + Water Mixtures at 298.15 K:	https://www.doi.org/10.1016/j.tca.2012.02.004
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume