(SS)- or (RR)-2,3-hexanediol

Inchi: InChI=1S/C6H14O2/c1-3-4-6(8)5(2)7/h5-8H,3-4H2,1-2H3/t5-,6-/m0/s1
InchiKey: QCIYAEYRVFUFAP-WDSKDSINSA-N
Formula: C6H14O2
SMILES: CCCC(O)C(C)O
Mol. weight [g/mol]: 118.17
CAS: 22520-19-0

Physical Properties

Property code	Value	Unit	Source
gf	-278.88	kJ/mol	Joback Method
hf	-482.19	kJ/mol	Joback Method
hfus	12.43	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	0.528		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	520.16	K	Joback Method
tc	683.21	K	Joback Method
tf	294.85 ± 0.30	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.68	J/mol×K	520.16	Joback Method
cpg	264.55	J/mol×K	547.34	Joback Method
cpg	273.06	J/mol×K	574.51	Joback Method
cpg	281.23	J/mol×K	601.69	Joback Method
cpg	289.05	J/mol×K	628.86	Joback Method
cpg	296.56	J/mol×K	656.04	Joback Method
cpg	303.74	J/mol×K	683.21	Joback Method
dvisc	0.6867154	Pa×s	249.02	Joback Method
dvisc	0.0457867	Pa×s	294.21	Joback Method

dvisc	0.0062787	Pa×s	339.40	Joback Method
dvisc	0.0013734	Pa×s	384.59	Joback Method
dvisc	0.0004135	Pa×s	429.78	Joback Method
dvisc	0.0001565	Pa×s	474.97	Joback Method
dvisc	0.0000701	Pa×s	520.16	Joback Method

Sources

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=C22520190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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