(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-/m1/s1
InchiKey: QCIYAEYRVFUFAP-WDSKDSINSA-N
Formula: C6H14O2
SMILES: CCC[C@@H](O)[C@@H](C)O
Mol. weight [g/mol]: 118.18

Physical Properties

Property code	Value	Unit	Source
af	0.6551		Cheméo Relay (1.0)
gf	-278.88	kJ/mol	Joback Method
hf	-472.12	kJ/mol	Cheméo Relay (1.0)
hfus	12.43	kJ/mol	Joback Method
hvap	69.91	kJ/mol	Cheméo Relay (1.0)
ie	10.22	eV	Cheméo Relay (1.0)
log10ws	-0.86		Cheméo Relay (1.0)
logp	0.528		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	475.56	K	Cheméo Relay (1.0)
tc	621.37	K	Cheméo Relay (1.0)
tf	294.85 ± 0.30	K	NIST Webbook
vc	0.424	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22520190&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
ie: Ionization energy
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