3,4-Hexanediol, 2,5-dimethyl-

Other names: 2,5-Dimethyl-3,4-hexanediol
Inchi: InChI=1S/C8H18O2/c1-5(2)7(9)8(10)6(3)4/h5-10H,1-4H3
InchiKey: UEGKGPFVYRPVCC-UHFFFAOYSA-N
Formula: C8H18O2
SMILES: CC(C)C(O)C(O)C(C)C
Mol. weight [g/mol]: 146.23
CAS: 22607-11-0

Physical Properties

Property code	Value	Unit	Source
gf	-266.92	kJ/mol	Joback Method
hf	-534.03	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	65.21	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.020		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	565.04	K	Joback Method
tc	732.17	K	Joback Method
tf	241.56	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.33	J/mol×K	565.04	Joback Method
cpg	357.37	J/mol×K	592.89	Joback Method
cpg	367.93	J/mol×K	620.75	Joback Method
cpg	378.03	J/mol×K	648.60	Joback Method
cpg	387.68	J/mol×K	676.46	Joback Method
cpg	396.91	J/mol×K	704.31	Joback Method
cpg	405.71	J/mol×K	732.17	Joback Method
dvisc	2.2442261	Pa×s	241.56	Joback Method

dvisc	0.0667226	Pa×s	295.47	Joback Method
dvisc	0.0058705	Pa×s	349.39	Joback Method
dvisc	0.0009892	Pa×s	403.30	Joback Method
dvisc	0.0002537	Pa×s	457.21	Joback Method
dvisc	0.0000867	Pa×s	511.13	Joback Method
dvisc	0.0000364	Pa×s	565.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22607110&Units=SI

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