3-Methylpent-2-ene-1,5-diol

Other names: 3-Methyl-1,5-pentenediol
Inchi: InChI=1S/C6H12O2/c1-6(2-4-7)3-5-8/h2,7-8H,3-5H2,1H3/b6-2+
InchiKey: TWUDHDJKTHYMGY-QHHAFSJGSA-N
Formula: C6H12O2
SMILES: CC(=CCO)CCO
Mol. weight [g/mol]: 116.16

Physical Properties

Property code	Value	Unit	Source
gf	-202.33	kJ/mol	Joback Method
hf	-364.20	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	62.35	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.307		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
ripol	1558.00		NIST Webbook
tb	525.08	K	Joback Method
tc	691.14	K	Joback Method
tf	259.98	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.34	J/mol×K	525.08	Joback Method
cpg	244.36	J/mol×K	552.76	Joback Method
cpg	252.02	J/mol×K	580.43	Joback Method
cpg	259.33	J/mol×K	608.11	Joback Method
cpg	266.31	J/mol×K	635.79	Joback Method
cpg	272.98	J/mol×K	663.46	Joback Method
cpg	279.36	J/mol×K	691.14	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=U191160&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume