1,2-Propanediol, 3-(dimethylamino)-

Other names: 3-(Dimethylamino)-1,2-propanediol
1-Dimethylamino-2,3-propanediol
3-dimethylaminopropane-1,2-diol
Inchi: InChI=1S/C5H13NO2/c1-6(2)3-5(8)4-7/h5,7-8H,3-4H2,1-2H3
InchiKey: QCMHUGYTOGXZIW-UHFFFAOYSA-N
Formula: C5H13NO2
SMILES: CN(C)CC(O)CO
Mol. weight [g/mol]: 119.16
CAS: 623-57-4

Physical Properties

Property code	Value	Unit	Source
gf	-174.08	kJ/mol	Joback Method
hf	-388.74	kJ/mol	Joback Method
hfus	16.38	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	0.88		Crippen Method
logp	-1.099		Crippen Method
mcvol	103.030	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	489.70	K	NIST Webbook
tc	669.87	K	Joback Method
tf	285.22	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.10	J/mol×K	510.16	Joback Method
cpg	253.57	J/mol×K	536.78	Joback Method
cpg	261.67	J/mol×K	563.40	Joback Method
cpg	269.42	J/mol×K	590.01	Joback Method
cpg	276.84	J/mol×K	616.63	Joback Method
cpg	283.92	J/mol×K	643.25	Joback Method

cpg	290.70	J/mol×K	669.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623574&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume