

2-Amino-1,3-propanediol

Other names:	1,3-dihydroxy-2-propylamine 1,3-dihydroxyisopropylamine 1,3-propanediol, 2-amino- 2-aminopropane-1,3-diol Serinol
Inchi:	InChI=1S/C3H9NO2/c4-3(1-5)2-6/h3,5-6H,1-2,4H2
InchiKey:	KJJPLEZQSCZCKE-UHFFFAOYSA-N
Formula:	C3H9NO2
SMILES:	NC(CO)CO
Mol. weight [g/mol]:	91.11
CAS:	534-03-2

Physical Properties

Property code	Value	Unit	Source
gf	-235.25	kJ/mol	Joback Method
hf	-381.20	kJ/mol	Joback Method
hfus	13.38	kJ/mol	Joback Method
hvap	65.88	kJ/mol	Joback Method
log10ws	0.85		Crippen Method
logp	-1.702		Crippen Method
mcvol	74.850	ml/mol	McGowan Method
pc	6328.92	kPa	Joback Method
tb	524.49	K	Joback Method
tc	698.04	K	Joback Method
tf	313.47	K	Joback Method
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.24	J/molxK	524.49	Joback Method
cpg	184.20	J/molxK	553.42	Joback Method
cpg	189.90	J/molxK	582.34	Joback Method
cpg	195.35	J/molxK	611.27	Joback Method

cpg	200.55	J/mol×K	640.19	Joback Method
cpg	205.52	J/mol×K	669.12	Joback Method
cpg	210.26	J/mol×K	698.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C534032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of CO2 in and Density, Viscosity, and Surface Tension of Aqueous Metho-1,3-propanediol (Serinol) Solutions:	https://www.doi.org/10.1021/je4008298
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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