3-Amino-1,2-propanediol

Other names:	1-Aminoglycerol
	1,2-Propanediol, 3-amino-
	1-Amino-2,3-propanediol
	2,3-Dihydroxypropylamine
	2,3-Propandiol-1-amine
	3-aminopropane-1,2-diol
Inchi:	InChI=1S/C3H9NO2/c4-1-3(6)2-5/h3,5-6H,1-2,4H2
InchiKey:	KQIGMPWTAHJUMN-UHFFFAOYSA-N
Formula:	C3H9NO2
SMILES:	NCC(O)CO
Mol. weight [g/mol]:	91.11
CAS:	616-30-8

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	537.50 ± 0.50	K	NIST Webbook
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/mol×K	524.49	Joback Method
cpg	184.20	J/mol×K	553.42	Joback Method
cpg	189.90	J/mol×K	582.34	Joback Method

cpg	195.35	J/mol×K	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	537.70	K	98.50	NIST Webbook
tbrp	385.50 ± 2.50	K	0.20	NIST Webbook
tbrp	369.50 ± 1.50	K	0.00	NIST Webbook
tbrp	436.00	K	2.00	NIST Webbook

Sources

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=C616308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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