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