

1-Propanol, 2-amino-, (.+/-.)-

Other names:	(.+/-.)-2-Amino-1-propanol (.+/-.)-Alaninol 1-Hydroxy-2-aminopropane 1-Methyl-2-hydroxyethylamine 1-Propanol, 2-amino- 1-Propanol, 2-amino-, DL- 2-Amino-1-propanol 2-Amino-2-methylethanol 2-Aminopropanol Alaninol DL-2-Amino-1-propanol DL-2-Aminopropanol DL-2-aminopropan-1-ol DL-Alaninol NSC 1360
Inchi:	InChI=1S/C3H9NO/c1-3(4)2-5/h3,5H,2,4H2,1H3
InchiKey:	BKMMTJMQCTUHRP-UHFFFAOYSA-N
Formula:	C3H9NO
SMILES:	CC(N)CO
Mol. weight [g/mol]:	75.11
CAS:	6168-72-5

Physical Properties

Property code	Value	Unit	Source
gf	-98.43	kJ/mol	Joback Method
hf	-228.97	kJ/mol	Joback Method
hfus	9.29	kJ/mol	Joback Method
hvap	49.20	kJ/mol	Joback Method
log10ws	0.11		Crippen Method
logp	-0.674		Crippen Method
mcvol	68.980	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
tb	447.70	K	NIST Webbook
tb	448.00	K	NIST Webbook
tc	613.40	K	Joback Method
tf	252.65	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.31	J/mol×K	432.31	Joback Method
cpg	149.06	J/mol×K	462.49	Joback Method
cpg	155.54	J/mol×K	492.67	Joback Method
cpg	161.74	J/mol×K	522.85	Joback Method
cpg	167.68	J/mol×K	553.03	Joback Method
cpg	173.36	J/mol×K	583.21	Joback Method
cpg	178.78	J/mol×K	613.40	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.33125e+01
Coeff. B	-6.38392e+03
Coeff. C	-6.54580e+01
Temperature range (K), min.	342.72
Temperature range (K), max.	420.10

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=C6168725&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

Latest version available from:

<https://www.cheméo.com/cid/66-943-2/1-Propanol-2-amino.pdf>

Generated by Cheméo on 2024-04-25 21:16:29.558064181 +0000 UTC m=+16369038.478641502.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.