

1-Butanol, 2-amino-

Other names:	1-(Hydroxymethyl)propylamine 1-Hydroxy-2-butylamine 2-Amino-1-butanol 2-Amino-1-hydroxybutane 2-Aminobutyl alcohol Butanol-2-amine 2-Aminobutan-1-ol 2-Amino-n-butyl alcohol 1-Butanol, 2-amino-, (.+/-)- (RS)-2-Amino-1-butanol DL-2-Aminobutanol 1-Hydroxy-sec-butylamine NSC 1068
Inchi:	InChI=1S/C4H11NO/c1-2-4(5)3-6/h4,6H,2-3,5H2,1H3
InchiKey:	JCBPETKZIGVZRE-UHFFFAOYSA-N
Formula:	C4H11NO
SMILES:	CCC(N)CO
Mol. weight [g/mol]:	89.14
CAS:	96-20-8

Physical Properties

Property code	Value	Unit	Source
gf	-90.01	kJ/mol	Joback Method
hf	-249.61	kJ/mol	Joback Method
hfus	11.88	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	-0.284		Crippen Method
mcvol	83.070	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
ripol	1547.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1544.00		NIST Webbook

ripol	1544.00		NIST Webbook
tb	455.19	K	Joback Method
tc	634.79	K	Joback Method
tf	263.92	K	Joback Method
vc	0.301	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.64	J/mol×K	455.19	Joback Method
cpg	187.68	J/mol×K	485.12	Joback Method
cpg	195.38	J/mol×K	515.06	Joback Method
cpg	202.76	J/mol×K	544.99	Joback Method
cpg	209.81	J/mol×K	574.92	Joback Method
cpg	216.56	J/mol×K	604.85	Joback Method
cpg	223.00	J/mol×K	634.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C96208&Units=SI

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

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