

1-Butanol, 2-amino-3-methyl-, (.+/-.)-

Other names:	(+)-2-Amino-3-methyl-1-butanol (±)-2-amino-3-methylbutan-1-ol
Inchi:	InChI=1S/C5H13NO/c1-4(2)5(6)3-7/h4-5,7H,3,6H2,1-2H3
InchiKey:	NWYYWIJOWOLJNR-UHFFFAOYSA-N
Formula:	C5H13NO
SMILES:	CC(C)C(N)CO
Mol. weight [g/mol]:	103.16
CAS:	16369-05-4

Physical Properties

Property code	Value	Unit	Source
gf	-84.03	kJ/mol	Joback Method
hf	-275.53	kJ/mol	Joback Method
hfus	10.94	kJ/mol	Joback Method
hvap	53.27	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	-0.038		Crippen Method
mvol	97.160	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	456.50 ± 2.50	K	NIST Webbook
tc	659.47	K	Joback Method
tf	260.19	K	Joback Method
vc	0.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.41	J/mol×K	477.63	Joback Method
cpg	228.88	J/mol×K	507.94	Joback Method
cpg	237.94	J/mol×K	538.24	Joback Method
cpg	246.60	J/mol×K	568.55	Joback Method
cpg	254.87	J/mol×K	598.85	Joback Method
cpg	262.75	J/mol×K	629.16	Joback Method
cpg	270.28	J/mol×K	659.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.20	K	1.00	NIST Webbook
tbrp	370.50 ± 2.50	K	1.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16369054&Units=SI
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

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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