

1-Butanol, 2-amino-, (S)-

Other names:	(+)-2-amino-1-butanol
Inchi:	InChI=1S/C4H11NO/c1-2-4(5)3-6/h4,6H,2-3,5H2,1H3/t4-/m1/s1
InchiKey:	JCBPETKZIGVZRE-SCSAIBSYSA-N
Formula:	C4H11NO
SMILES:	CCC(N)CO
Mol. weight [g/mol]:	89.14
CAS:	5856-62-2

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
tb	446.20	K	NIST Webbook
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/molxK	455.19	Joback Method
cpg	187.68	J/molxK	485.12	Joback Method
cpg	195.38	J/molxK	515.06	Joback Method
cpg	202.76	J/molxK	544.99	Joback Method
cpg	209.81	J/molxK	574.92	Joback Method
cpg	216.56	J/molxK	604.85	Joback Method
cpg	223.00	J/molxK	634.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C5856622&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
h vap:	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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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