

Butyrohydroxamic acid, 2-amino-

Inchi:	InChI=1S/C4H10N2O2/c1-2-3(5)4(7)6-8/h3,8H,2,5H2,1H3,(H,6,7)
InchiKey:	TYTVEXBKMJEECD-UHFFFAOYSA-N
Formula:	C4H10N2O2
SMILES:	CCC(N)C(=O)NO
Mol. weight [g/mol]:	118.13
CAS:	36212-74-5

Physical Properties

Property code	Value	Unit	Source
gf	-129.54	kJ/mol	Joback Method
hf	-308.72	kJ/mol	Joback Method
hfus	18.58	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	0.34		Crippen Method
logp	-0.771		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	5335.72	kPa	Joback Method
tb	559.23	K	Joback Method
tc	750.23	K	Joback Method
tf	366.51	K	Joback Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.16	J/molxK	559.23	Joback Method
cpg	237.98	J/molxK	591.06	Joback Method
cpg	245.40	J/molxK	622.90	Joback Method
cpg	252.43	J/molxK	654.73	Joback Method
cpg	259.08	J/molxK	686.56	Joback Method
cpg	265.37	J/molxK	718.40	Joback Method
cpg	271.30	J/molxK	750.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36212745&Units=SI&Mask=3FFF
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
mccvol:	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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