

«beta»-Alanyl-«beta»-alanine

Inchi:	InChI=1S/C6H12N2O3/c1-4(6(10)11)8-5(9)2-3-7/h4H,2-3,7H2,1H3,(H,8,9)(H,10,11)
InchiKey:	OSOCQWFTTAPWEK-UHFFFAOYSA-N
Formula:	C6H12N2O3
SMILES:	CC(NC(=O)CCN)C(=O)O
Mol. weight [g/mol]:	160.17
CAS:	34322-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-241.62	kJ/mol	Joback Method
hf	-462.58	kJ/mol	Joback Method
hfus	25.36	kJ/mol	Joback Method
hvap	75.81	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-1.075		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	658.86	K	Joback Method
tc	852.80	K	Joback Method
tf	438.98	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.70	J/molxK	658.86	Joback Method
cpg	339.36	J/molxK	691.18	Joback Method
cpg	347.52	J/molxK	723.51	Joback Method
cpg	355.19	J/molxK	755.83	Joback Method
cpg	362.40	J/molxK	788.16	Joback Method
cpg	369.14	J/molxK	820.48	Joback Method
cpg	375.45	J/molxK	852.80	Joback Method
cps	196.00	J/molxK	298.00	NIST Webbook
cps	196.00	J/molxK	298.00	NIST Webbook

Sources

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=C34322877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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