

«beta»-Alanylglycine

Inchi:	InChI=1S/C5H10N2O3/c6-2-1-4(8)7-3-5(9)10/h1-3,6H2,(H,7,8)(H,9,10)
InchiKey:	QDHYJVJAGQLHBA-UHFFFAOYSA-N
Formula:	C5H10N2O3
SMILES:	NCCC(=O)NCC(=O)O
Mol. weight [g/mol]:	146.14
CAS:	2672-88-0

Physical Properties

Property code	Value	Unit	Source
gf	-247.60	kJ/mol	Joback Method
hf	-436.66	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hvap	73.97	kJ/mol	Joback Method
log10ws	0.59		Crippen Method
logp	-1.464		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	636.42	K	Joback Method
tc	829.14	K	Joback Method
tf	442.71	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.27	J/molxK	797.02	Joback Method
cpg	283.14	J/molxK	636.42	Joback Method
cpg	290.81	J/molxK	668.54	Joback Method
cpg	298.04	J/molxK	700.66	Joback Method
cpg	304.85	J/molxK	732.78	Joback Method
cpg	311.26	J/molxK	764.90	Joback Method
cpg	322.89	J/molxK	829.14	Joback Method
cps	168.00	J/molxK	298.00	NIST Webbook
hfust	56.60	kJ/mol	507.95	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2672880&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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