Methyl acetylglycinate

Other names:	Methyl N-acetylglycinate
	Methyl N-acetylglycine
	N-Acetylglycine methyl ester
	CH3C(O)NHCH2C(O)OCH3
	Acetylglycine, methyl ester
Inchi:	InChI=1S/C5H9NO3/c1-4(7)6-3-5(8)9-2/h3H2,1-2H3,(H,6,7)
InchiKey:	RFNODQARGNZURK-UHFFFAOYSA-N
Formula:	C5H9NO3
SMILES:	COC(=O)CNC(C)=O
Mol. weight [g/mol]:	131.13
CAS:	1117-77-7

Physical Properties

Property code	Value	Unit	Source
affp	892.00	kJ/mol	NIST Webbook
basg	861.00	kJ/mol	NIST Webbook
gf	-282.23	kJ/mol	Joback Method
hf	-450.44	kJ/mol	Joback Method
hfus	18.19	kJ/mol	Joback Method
hvap	49.06	kJ/mol	Joback Method
log10ws	0.26		Crippen Method
logp	-0.705		Crippen Method
mcvol	100.300	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1137.60		NIST Webbook
tb	494.13	K	Joback Method
tc	687.46	K	Joback Method
tf	320.86	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	214.78	J/mol×K	494.13	Joback Method
cpg	223.59	J/mol×K	526.35	Joback Method
cpg	232.04	J/mol×K	558.57	Joback Method
cpg	240.14	J/mol×K	590.80	Joback Method
cpg	247.88	J/mol×K	623.02	Joback Method
cpg	255.26	J/mol×K	655.24	Joback Method
cpg	262.27	J/mol×K	687.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1117777&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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