Glycine, N-acetyl-, methyl ester

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

Physical Properties

Property code	Value	Unit	Source
af	0.5055		Cheméo Relay (1.0)
affp	892.00	kJ/mol	NIST Webbook
basg	861.00	kJ/mol	NIST Webbook
hf	-578.22	kJ/mol	Cheméo Relay (1.0)
hfus	18.19	kJ/mol	Joback Method
hvap	65.03	kJ/mol	Cheméo Relay (1.0)
ie	9.42	eV	Cheméo Relay (1.0)
log10ws	-0.04		Cheméo Relay (1.0)
logp	-0.705		Crippen Method
mcvol	100.300	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1137.60		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
tb	494.20	K	Cheméo Relay (1.0)
tc	661.93	K	Cheméo Relay (1.0)
tf	296.99	K	Cheméo Relay (1.0)
vc	0.372	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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