Glycine, methyl ester

Other names:	NH2CH2COOCH3
	methyl glycinate
Inchi:	InChI=1S/C3H7NO2/c1-6-3(5)2-4/h2,4H2,1H3
InchiKey:	KQSSATDQUYCRGS-UHFFFAOYSA-N
Formula:	C3H7NO2
SMILES:	COC(=O)CN
Mol. weight [g/mol]:	89.09
CAS:	616-34-2

Physical Properties

Property code	Value	Unit	Source
gf	-193.09	kJ/mol	Joback Method
hf	-316.26	kJ/mol	Joback Method
hfus	11.51	kJ/mol	Joback Method
hvap	42.07	kJ/mol	Joback Method
ie	9.80	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	0.63		Crippen Method
logp	-0.882		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	749.00		NIST Webbook
tb	416.86	K	Joback Method
tc	613.38	K	Joback Method
tf	278.99	K	Joback Method
vc	0.257	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.41	J/mol×K	416.86	Joback Method
cpg	142.88	J/mol×K	449.61	Joback Method
cpg	149.16	J/mol×K	482.37	Joback Method
cpg	155.23	J/mol×K	515.12	Joback Method

cpg	161.10	J/mol×K	547.87	Joback Method
cpg	166.75	J/mol×K	580.63	Joback Method
cpg	172.18	J/mol×K	613.38	Joback Method

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=C616342&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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