Methacrylglycine, methyl ester

Inchi: InChI=1S/C8H13NO3/c1-6(2)4-7(10)9-5-8(11)12-3/h1,4-5H2,2-3H3,(H,9,10)
InchiKey: TZSHCLFMEXZCRJ-UHFFFAOYSA-N
Formula: C8H13NO3
SMILES: C=C(C)CC(=O)NCC(=O)OC
Mol. weight [g/mol]: 171.19

Physical Properties

Property code	Value	Unit	Source
gf	-177.68	kJ/mol	Joback Method
hf	-396.72	kJ/mol	Joback Method
hfus	23.37	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.242		Crippen Method
mcvol	138.270	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	559.33	K	Joback Method
tc	752.54	K	Joback Method
tf	338.95	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.66	J/mol×K	559.33	Joback Method
cpg	337.05	J/mol×K	591.53	Joback Method
cpg	347.89	J/mol×K	623.73	Joback Method
cpg	358.19	J/mol×K	655.93	Joback Method
cpg	367.96	J/mol×K	688.14	Joback Method
cpg	377.21	J/mol×K	720.34	Joback Method
cpg	385.94	J/mol×K	752.54	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=R245571&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
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