Acrylylglycine, methyl ester

Inchi: InChI=1S/C6H9NO3/c1-3-5(8)7-4-6(9)10-2/h3H,1,4H2,2H3,(H,7,8)
InchiKey: GPXGYCOUOXWPOW-UHFFFAOYSA-N
Formula: C6H9NO3
SMILES: C=CC(=O)NCC(=O)OC
Mol. weight [g/mol]: 143.14

Physical Properties

Property code	Value	Unit	Source
gf	-185.97	kJ/mol	Joback Method
hf	-345.65	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	50.62	kJ/mol	Joback Method
log10ws	-0.01		Crippen Method
logp	-0.538		Crippen Method
mcvol	110.090	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
tb	513.69	K	Joback Method
tc	708.54	K	Joback Method
tf	330.37	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.36	J/mol×K	513.69	Joback Method
cpg	247.60	J/mol×K	546.17	Joback Method
cpg	256.41	J/mol×K	578.64	Joback Method
cpg	264.80	J/mol×K	611.12	Joback Method
cpg	272.78	J/mol×K	643.59	Joback Method
cpg	280.34	J/mol×K	676.07	Joback Method
cpg	287.49	J/mol×K	708.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R245531&Units=SI
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

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