Vinylacetylglycine, methyl ester

Inchi: InChI=1S/C7H11NO3/c1-3-4-6(9)8-5-7(10)11-2/h3H,1,4-5H2,2H3,(H,8,9)
InchiKey: MGICTTHNDAIMFI-UHFFFAOYSA-N
Formula: C7H11NO3
SMILES: C=CCC(=O)NCC(=O)OC
Mol. weight [g/mol]: 157.17

Physical Properties

Property code	Value	Unit	Source
gf	-177.55	kJ/mol	Joback Method
hf	-366.29	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	52.84	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	-0.148		Crippen Method
mcvol	124.180	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1444.00		NIST Webbook
tb	536.57	K	Joback Method
tc	728.94	K	Joback Method
tf	341.64	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.15	J/mol×K	536.57	Joback Method
cpg	291.45	J/mol×K	568.63	Joback Method
cpg	301.26	J/mol×K	600.69	Joback Method
cpg	310.60	J/mol×K	632.76	Joback Method
cpg	319.47	J/mol×K	664.82	Joback Method
cpg	327.88	J/mol×K	696.88	Joback Method
cpg	335.82	J/mol×K	728.94	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=R245704&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