Methylenecyclopropylacetylglycine, methyl ester

Inchi: InChI=1S/C9H13NO3/c1-6-3-7(6)4-8(11)10-5-9(12)13-2/h7H,1,3-5H2,2H3,(H,10,11)
InchiKey: QTZVDFGXRKEEIC-UHFFFAOYSA-N
Formula: C9H13NO3
SMILES: C=C1CC1CC(=O)NCC(=O)OC
Mol. weight [g/mol]: 183.20

Physical Properties

Property code	Value	Unit	Source
gf	-134.72	kJ/mol	Joback Method
hf	-375.96	kJ/mol	Joback Method
hfus	25.53	kJ/mol	Joback Method
hvap	58.04	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	0.242		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
tb	591.55	K	Joback Method
tc	789.84	K	Joback Method
tf	397.56	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.79	J/mol×K	591.55	Joback Method
cpg	368.81	J/mol×K	624.60	Joback Method
cpg	380.18	J/mol×K	657.65	Joback Method
cpg	390.92	J/mol×K	690.70	Joback Method
cpg	401.05	J/mol×K	723.75	Joback Method
cpg	410.59	J/mol×K	756.79	Joback Method
cpg	419.56	J/mol×K	789.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R245586&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