Glycine, N-pivaloyl-, methyl ester

Inchi: InChI=1S/C8H15NO3/c1-8(2,3)7(11)9-5-6(10)12-4/h5H2,1-4H3,(H,9,11)
InchiKey: LQVNCECMNJKXEJ-UHFFFAOYSA-N
Formula: C8H15NO3
SMILES: COC(=O)CNC(=O)C(C)(C)C
Mol. weight [g/mol]: 173.21

Physical Properties

Property code	Value	Unit	Source
gf	-254.13	kJ/mol	Joback Method
hf	-521.11	kJ/mol	Joback Method
hfus	18.55	kJ/mol	Joback Method
hvap	54.44	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	0.322		Crippen Method
mcvol	142.570	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
tb	559.54	K	Joback Method
tc	756.74	K	Joback Method
tf	357.09	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.94	J/mol×K	559.54	Joback Method
cpg	361.53	J/mol×K	592.41	Joback Method
cpg	373.43	J/mol×K	625.27	Joback Method
cpg	384.66	J/mol×K	658.14	Joback Method
cpg	395.25	J/mol×K	691.00	Joback Method
cpg	405.21	J/mol×K	723.87	Joback Method
cpg	414.57	J/mol×K	756.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299742&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