Glycine, N-methyl-N-allyloxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C11H19NO4/c1-5-6-15-11(14)12(4)7-10(13)16-8-9(2)3/h5,9H,1,6-8H2,2-4H3
InchiKey: XBXPLCYDEGTNOJ-UHFFFAOYSA-N
Formula: C11H19NO4
SMILES: C=CCOC(=O)N(C)CC(=O)OCC(C)C
Mol. weight [g/mol]: 229.27

Physical Properties

Property code	Value	Unit	Source
gf	-229.92	kJ/mol	Joback Method
hf	-572.29	kJ/mol	Joback Method
hfus	28.04	kJ/mol	Joback Method
hvap	59.38	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.440		Crippen Method
mcvol	186.410	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1477.00		NIST Webbook
tb	612.34	K	Joback Method
tc	795.27	K	Joback Method
tf	373.76	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.49	J/mol×K	612.34	Joback Method
cpg	495.55	J/mol×K	642.83	Joback Method
cpg	508.94	J/mol×K	673.32	Joback Method
cpg	521.65	J/mol×K	703.81	Joback Method
cpg	533.71	J/mol×K	734.29	Joback Method
cpg	545.11	J/mol×K	764.78	Joback Method
cpg	555.86	J/mol×K	795.27	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U320587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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