Glycine, N-methyl-N-allyloxycarbonyl-, heptyl ester

Inchi: InChI=1S/C14H25NO4/c1-4-6-7-8-9-11-18-13(16)12-15(3)14(17)19-10-5-2/h5H,2,4,6-12

InchiKey: MIJBJBIEKIBXBZ-UHFFFAOYSA-N

Formula: C14H25NO4

SMILES: C=CCOC(=O)N(C)CC(=O)OCCCCCCC

Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
gf	-202.22	kJ/mol	Joback Method
hf	-628.93	kJ/mol	Joback Method
hfus	39.33	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.754		Crippen Method
mcvol	228.680	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	681.42	K	Joback Method
tc	858.67	K	Joback Method
tf	422.57	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.67	J/mol×K	681.42	Joback Method
cpg	654.05	J/mol×K	710.96	Joback Method
cpg	668.66	J/mol×K	740.50	Joback Method
cpg	682.52	J/mol×K	770.04	Joback Method
cpg	695.64	J/mol×K	799.58	Joback Method
cpg	708.04	J/mol×K	829.12	Joback Method
cpg	719.73	J/mol×K	858.67	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=U320591&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