Glycine, N-methyl-N-allyloxycarbonyl-, pentyl ester

Inchi: InChI=1S/C12H21NO4/c1-4-6-7-9-16-11(14)10-13(3)12(15)17-8-5-2/h5H,2,4,6-10H2,1,3

InchiKey: RRAHMMVWLIPAGJ-UHFFFAOYSA-N

Formula: C12H21NO4

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

Mol. weight [g/mol]: 243.30

Physical Properties

Property code	Value	Unit	Source
gf	-219.06	kJ/mol	Joback Method
hf	-587.65	kJ/mol	Joback Method
hfus	34.15	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.974		Crippen Method
mcvol	200.500	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1592.00		NIST Webbook
tb	635.66	K	Joback Method
tc	814.29	K	Joback Method
tf	400.03	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.20	J/mol×K	635.66	Joback Method
cpg	546.57	J/mol×K	665.43	Joback Method
cpg	560.26	J/mol×K	695.20	Joback Method
cpg	573.26	J/mol×K	724.98	Joback Method
cpg	585.60	J/mol×K	754.75	Joback Method
cpg	597.27	J/mol×K	784.52	Joback Method
cpg	608.30	J/mol×K	814.29	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=U320588&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