Glycine, N-methyl-N-allyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C18H33NO4/c1-4-6-7-8-9-10-11-12-13-15-22-17(20)16-19(3)18(21)23-14-5-2/h5H,2,4,6-16H2,1,3H3

InchiKey: TXDRUHURSAJNCA-UHFFFAOYSA-N

Formula: C18H33NO4

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

Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
gf	-168.54	kJ/mol	Joback Method
hf	-711.49	kJ/mol	Joback Method
hfus	49.69	kJ/mol	Joback Method
hvap	75.35	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.315		Crippen Method
mcvol	285.040	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	2098.00		NIST Webbook
tb	772.94	K	Joback Method
tc	953.18	K	Joback Method
tf	467.65	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.90	J/mol×K	772.94	Joback Method
cpg	882.94	J/mol×K	802.98	Joback Method
cpg	899.05	J/mol×K	833.02	Joback Method
cpg	914.25	J/mol×K	863.06	Joback Method
cpg	928.55	J/mol×K	893.10	Joback Method
cpg	941.98	J/mol×K	923.14	Joback Method
cpg	954.56	J/mol×K	953.18	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=U320595&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