Glycine, N-methyl-N-allyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C15H27NO4/c1-4-6-7-8-9-10-12-19-14(17)13-16(3)15(18)20-11-5-2/h5H,2,4,6-

InchiKey: ZMEBVGWCUAPVDG-UHFFFAOYSA-N

Formula: C15H27NO4

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

Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
gf	-193.80	kJ/mol	Joback Method
hf	-649.57	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.144		Crippen Method
mcvol	242.770	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
tb	704.30	K	Joback Method
tc	881.49	K	Joback Method
tf	433.84	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.82	J/mol×K	704.30	Joback Method
cpg	709.64	J/mol×K	733.83	Joback Method
cpg	724.66	J/mol×K	763.36	Joback Method
cpg	738.89	J/mol×K	792.90	Joback Method
cpg	752.34	J/mol×K	822.43	Joback Method
cpg	765.04	J/mol×K	851.96	Joback Method
cpg	776.99	J/mol×K	881.49	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=U320592&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