Glycine, N-methyl-N-allyloxycarbonyl-, octadecyl ester

Inchi: InChI=1S/C25H47NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-29-24(27)23-
InchiKey: SPLCOMITFUNDHO-UHFFFAOYSA-N
Formula: C25H47NO4
SMILES: C=CCOC(=O)N(C)CC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
gf	-109.60	kJ/mol	Joback Method
hf	-855.97	kJ/mol	Joback Method
hfus	67.82	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	7.045		Crippen Method
mcvol	383.670	ml/mol	McGowan Method
pc	822.90	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	933.10	K	Joback Method
tc	1146.70	K	Joback Method
tf	546.54	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1296.51	J/mol×K	933.10	Joback Method
cpg	1316.94	J/mol×K	968.70	Joback Method
cpg	1335.87	J/mol×K	1004.30	Joback Method
cpg	1353.35	J/mol×K	1039.90	Joback Method
cpg	1369.45	J/mol×K	1075.50	Joback Method
cpg	1384.22	J/mol×K	1111.10	Joback Method
cpg	1397.72	J/mol×K	1146.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320600&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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