Glycine, N-methyl-N-allyloxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C24H45NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-28-23(26)22-25(
InchiKey: SEHUSDUMAUOKJP-UHFFFAOYSA-N
Formula: C24H45NO4
SMILES: C=CCOC(=O)N(C)CC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 411.62

Physical Properties

Property code	Value	Unit	Source
gf	-118.02	kJ/mol	Joback Method
hf	-835.33	kJ/mol	Joback Method
hfus	65.23	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.655		Crippen Method
mcvol	369.580	ml/mol	McGowan Method
pc	870.16	kPa	Joback Method
rinpol	2625.00		NIST Webbook
tb	910.22	K	Joback Method
tc	1116.20	K	Joback Method
tf	535.27	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.10	J/mol×K	910.22	Joback Method
cpg	1252.93	J/mol×K	944.55	Joback Method
cpg	1271.38	J/mol×K	978.88	Joback Method
cpg	1288.50	J/mol×K	1013.21	Joback Method
cpg	1304.33	J/mol×K	1047.54	Joback Method
cpg	1318.92	J/mol×K	1081.87	Joback Method
cpg	1332.33	J/mol×K	1116.20	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=U320599&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