

Glycine, N-methyl-N-allyloxycarbonyl-, hexadecyl ester

Inchi:	InChI=1S/C23H43NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-20-27-22(25)21-24(3)2
InchiKey:	JXSFVUXQEBXUEB-UHFFFAOYSA-N
Formula:	C23H43NO4
SMILES:	C=CCOC(=O)N(C)CC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	397.59

Physical Properties

Property code	Value	Unit	Source
gf	-126.44	kJ/mol	Joback Method
hf	-814.69	kJ/mol	Joback Method
hfus	62.64	kJ/mol	Joback Method
hvap	86.48	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.265		Crippen Method
mcvol	355.490	ml/mol	McGowan Method
pc	921.62	kPa	Joback Method
rinpol	2537.00		NIST Webbook
tb	887.34	K	Joback Method
tc	1086.77	K	Joback Method
tf	524.00	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.22	J/molxK	887.34	Joback Method
cpg	1189.51	J/molxK	920.58	Joback Method
cpg	1207.51	J/molxK	953.82	Joback Method
cpg	1224.27	J/molxK	987.05	Joback Method
cpg	1239.84	J/molxK	1020.29	Joback Method
cpg	1254.25	J/molxK	1053.53	Joback Method
cpg	1267.55	J/molxK	1086.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U320598&Units=SI

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
mccvol:	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

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