

Glycine, N-methyl-N-allyloxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C9H15NO4/c1-4-6-14-9(12)10(3)7-8(11)13-5-2/h4H,1,5-7H2,2-3H3
InchiKey:	YEMXMCZWBCOZQF-UHFFFAOYSA-N
Formula:	C9H15NO4
SMILES:	C=CCOC(=O)N(C)CC(=O)OCC
Mol. weight [g/mol]:	201.22

Physical Properties

Property code	Value	Unit	Source
gf	-244.32	kJ/mol	Joback Method
hf	-525.73	kJ/mol	Joback Method
hfus	26.38	kJ/mol	Joback Method
hvap	55.31	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	0.804		Crippen Method
mcvol	158.230	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
tb	567.02	K	Joback Method
tc	750.18	K	Joback Method
tf	366.22	K	Joback Method
vc	0.587	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.48	J/mol×K	567.02	Joback Method
cpg	395.86	J/mol×K	597.55	Joback Method
cpg	407.69	J/mol×K	628.07	Joback Method
cpg	418.95	J/mol×K	658.60	Joback Method
cpg	429.66	J/mol×K	689.13	Joback Method
cpg	439.83	J/mol×K	719.65	Joback Method
cpg	449.45	J/mol×K	750.18	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U320586&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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