l-Norvaline, N-allyloxycarbonyl-, ethyl ester

Inchi: InChI=1S/C11H19NO4/c1-4-7-9(10(13)15-6-3)12-11(14)16-8-5-2/h5,9H,2,4,6-8H2,1,3H3
InchiKey: WQPPQGMDMDHDOW-UHFFFAOYSA-N
Formula: C11H19NO4
SMILES: C=CCOC(=O)NC(CCC)C(=O)OCC
Mol. weight [g/mol]: 229.27

Physical Properties

Property code	Value	Unit	Source
gf	-251.31	kJ/mol	Joback Method
hf	-586.35	kJ/mol	Joback Method
hfus	30.12	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.630		Crippen Method
mcvol	186.410	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
tb	650.07	K	Joback Method
tc	836.42	K	Joback Method
tf	393.95	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.91	J/mol×K	650.07	Joback Method
cpg	510.43	J/mol×K	681.13	Joback Method
cpg	523.27	J/mol×K	712.19	Joback Method
cpg	535.44	J/mol×K	743.24	Joback Method
cpg	546.95	J/mol×K	774.30	Joback Method
cpg	557.79	J/mol×K	805.36	Joback Method
cpg	567.96	J/mol×K	836.42	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=U320744&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

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