DL-Alanine, N-methyl-N-(vinyloxycarbonyl)-, hexyl ester

Inchi: InChI=1S/C13H23NO4/c1-5-7-8-9-10-18-12(15)11(3)14(4)13(16)17-6-2/h6,11H,2,5,7-10H

InchiKey: MRLXPDBXNZOTAQ-UHFFFAOYSA-N

Formula: C13H23NO4

SMILES: C=COC(=O)N(C)C(C)C(=O)OCCCCCC

Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
gf	-213.08	kJ/mol	Joback Method
hf	-613.57	kJ/mol	Joback Method
hfus	33.22	kJ/mol	Joback Method
hvap	63.83	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.710		Crippen Method
mcvol	214.590	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	1641.00		NIST Webbook
rinpol	1641.00		NIST Webbook
tb	658.10	K	Joback Method
tc	838.44	K	Joback Method
tf	396.30	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.22	J/mol×K	658.10	Joback Method
cpg	600.37	J/mol×K	688.16	Joback Method
cpg	614.77	J/mol×K	718.21	Joback Method
cpg	628.42	J/mol×K	748.27	Joback Method
cpg	641.34	J/mol×K	778.33	Joback Method
cpg	653.54	J/mol×K	808.38	Joback Method
cpg	665.03	J/mol×K	838.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392752&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