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

Inchi: InChI=1S/C14H25NO4/c1-5-7-8-9-10-11-19-13(16)12(3)15(4)14(17)18-6-2/h6,12H,2,5,7-

InchiKey: HDGWWKCTVGFFLH-UHFFFAOYSA-N

Formula: C14H25NO4

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

Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
gf	-204.66	kJ/mol	Joback Method
hf	-634.21	kJ/mol	Joback Method
hfus	35.81	kJ/mol	Joback Method
hvap	66.06	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.100		Crippen Method
mcvol	228.680	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
tb	680.98	K	Joback Method
tc	860.58	K	Joback Method
tf	407.57	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.14	J/mol×K	680.98	Joback Method
cpg	654.75	J/mol×K	710.91	Joback Method
cpg	669.57	J/mol×K	740.85	Joback Method
cpg	683.61	J/mol×K	770.78	Joback Method
cpg	696.88	J/mol×K	800.71	Joback Method
cpg	709.40	J/mol×K	830.65	Joback Method
cpg	721.18	J/mol×K	860.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392753&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

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