

DL-Alanine, N-methyl-N-(vinylloxycarbonyl)-, butyl ester

Inchi: InChI=1S/C11H19NO4/c1-5-7-8-16-10(13)9(3)12(4)11(14)15-6-2/h6,9H,2,5,7-8H2,1,3-4H
InchiKey: LHQDHKUIVPRYIM-UHFFFAOYSA-N
Formula: C11H19NO4
SMILES: C=COC(=O)N(C)C(C)C(=O)OCCCC
Mol. weight [g/mol]: 229.27

Physical Properties

Property code	Value	Unit	Source
gf	-229.92	kJ/mol	Joback Method
hf	-572.29	kJ/mol	Joback Method
hfus	28.04	kJ/mol	Joback Method
hvap	59.38	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.930		Crippen Method
mcvol	186.410	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	612.34	K	Joback Method
tc	795.27	K	Joback Method
tf	373.76	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.49	J/mol×K	612.34	Joback Method
cpg	495.55	J/mol×K	642.83	Joback Method
cpg	508.94	J/mol×K	673.32	Joback Method
cpg	521.65	J/mol×K	703.81	Joback Method
cpg	533.71	J/mol×K	734.29	Joback Method
cpg	545.11	J/mol×K	764.78	Joback Method
cpg	555.86	J/mol×K	795.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392751&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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