DL-Alanine, N-methyl-N-(2-benzyloxyethoxycarbonyl)-, decyl ester

Inchi: InChI=1S/C24H39NO5/c1-4-5-6-7-8-9-10-14-17-29-23(26)21(2)25(3)24(27)30-19-18-28-
InchiKey: VBJGABJCXGDEBF-UHFFFAOYSA-N
Formula: C24H39NO5
SMILES: CCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 421.57

Physical Properties

Property code	Value	Unit	Source
gf	-200.89	kJ/mol	Joback Method
hf	-861.73	kJ/mol	Joback Method
hfus	58.22	kJ/mol	Joback Method
hvap	93.67	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.344		Crippen Method
mcvol	355.990	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2876.00		NIST Webbook
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tb	962.20	K	Joback Method
tc	1178.01	K	Joback Method
tf	570.68	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1193.78	J/mol×K	962.20	Joback Method
cpg	1210.29	J/mol×K	998.17	Joback Method
cpg	1225.26	J/mol×K	1034.14	Joback Method
cpg	1238.74	J/mol×K	1070.10	Joback Method
cpg	1250.75	J/mol×K	1106.07	Joback Method
cpg	1261.35	J/mol×K	1142.04	Joback Method
cpg	1270.58	J/mol×K	1178.01	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=U392694&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
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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