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

Inchi: InChI=1S/C25H41NO5/c1-4-5-6-7-8-9-10-11-15-18-30-24(27)22(2)26(3)25(28)31-20-19-
InchiKey: KJSYYUFUYSKMCD-UHFFFAOYSA-N
Formula: C25H41NO5
SMILES: CCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 435.60

Physical Properties

Property code	Value	Unit	Source
gf	-192.47	kJ/mol	Joback Method
hf	-882.37	kJ/mol	Joback Method
hfus	60.81	kJ/mol	Joback Method
hvap	95.90	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.734		Crippen Method
mcvol	370.080	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
rinpol	2979.00		NIST Webbook
rinpol	2979.00		NIST Webbook
tb	985.08	K	Joback Method
tc	1206.64	K	Joback Method
tf	581.95	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1255.72	J/mol×K	985.08	Joback Method
cpg	1272.45	J/mol×K	1022.01	Joback Method
cpg	1287.53	J/mol×K	1058.93	Joback Method
cpg	1301.01	J/mol×K	1095.86	Joback Method
cpg	1312.96	J/mol×K	1132.78	Joback Method
cpg	1323.40	J/mol×K	1169.71	Joback Method
cpg	1332.40	J/mol×K	1206.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392695&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