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

Inchi: InChI=1S/C22H35NO5/c1-4-5-6-7-8-12-15-27-21(24)19(2)23(3)22(25)28-17-16-26-18-20
InchiKey: UZVZALCXDBSKSZ-UHFFFAOYSA-N
Formula: C22H35NO5
SMILES: CCCCCCCCOC(=O)C(C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 393.52

Physical Properties

Property code	Value	Unit	Source
gf	-217.73	kJ/mol	Joback Method
hf	-820.45	kJ/mol	Joback Method
hfus	53.04	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.564		Crippen Method
mcvol	327.810	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	916.44	K	Joback Method
tc	1123.78	K	Joback Method
tf	548.14	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1071.22	J/mol×K	916.44	Joback Method
cpg	1087.37	J/mol×K	951.00	Joback Method
cpg	1102.14	J/mol×K	985.55	Joback Method
cpg	1115.56	J/mol×K	1020.11	Joback Method
cpg	1127.67	J/mol×K	1054.67	Joback Method
cpg	1138.49	J/mol×K	1089.23	Joback Method
cpg	1148.07	J/mol×K	1123.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392692&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