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

InChI: InChI=1S/C23H29NO6/c1-19(22(25)29-15-13-27-17-20-9-5-3-6-10-20)24(2)23(26)30-16-
InChIKey: DIAMMBHSEGNBBB-UHFFFAOYSA-N
Formula: C23H29NO6
SMILES: CC(C(=O)OCCOCc1ccccc1)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 415.48

Physical Properties

Property code	Value	Unit	Source
gf	-201.90	kJ/mol	Joback Method
hf	-736.78	kJ/mol	Joback Method
hfus	50.86	kJ/mol	Joback Method
hvap	96.13	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.420		Crippen Method
mcvol	324.010	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	3027.00		NIST Webbook
rinpol	3027.00		NIST Webbook
tb	988.42	K	Joback Method
tc	1214.41	K	Joback Method
tf	608.06	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1055.43	J/mol×K	988.42	Joback Method
cpg	1068.03	J/mol×K	1026.08	Joback Method
cpg	1078.99	J/mol×K	1063.75	Joback Method
cpg	1088.36	J/mol×K	1101.41	Joback Method
cpg	1096.17	J/mol×K	1139.08	Joback Method
cpg	1102.45	J/mol×K	1176.74	Joback Method
cpg	1107.25	J/mol×K	1214.41	Joback Method

Sources

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=U392698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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