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

Inchi: InChI=1S/C18H27NO5/c1-14(2)12-24-17(20)15(3)19(4)18(21)23-11-10-22-13-16-8-6-5-7

InchiKey: HKVBQCYIRZVLLH-UHFFFAOYSA-N

Formula: C18H27NO5

SMILES: CC(C)COC(=O)C(C)N(C)C(=O)OCCOCc1ccccc1

Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
gf	-253.85	kJ/mol	Joback Method
hf	-743.17	kJ/mol	Joback Method
hfus	39.15	kJ/mol	Joback Method
hvap	79.93	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.859		Crippen Method
mcvol	271.450	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	824.48	K	Joback Method
tc	1027.23	K	Joback Method
tf	488.06	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.61	J/mol×K	824.48	Joback Method
cpg	849.25	J/mol×K	858.27	Joback Method
cpg	863.71	J/mol×K	892.06	Joback Method
cpg	876.98	J/mol×K	925.86	Joback Method
cpg	889.10	J/mol×K	959.65	Joback Method
cpg	900.08	J/mol×K	993.44	Joback Method
cpg	909.95	J/mol×K	1027.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392687&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