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

Inchi: InChI=1S/C18H27NO5/c1-4-5-11-23-17(20)15(2)19(3)18(21)24-13-12-22-14-16-9-7-6-8-
InchiKey: BTUSMTZVYYIQKC-UHFFFAOYSA-N
Formula: C18H27NO5
SMILES: CCCCOC(=O)C(C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 337.41

Physical Properties

Property code	Value	Unit	Source
gf	-251.41	kJ/mol	Joback Method
hf	-737.89	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	80.31	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.003		Crippen Method
mcvol	271.450	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
tb	824.92	K	Joback Method
tc	1025.63	K	Joback Method
tf	503.06	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.08	J/mol×K	824.92	Joback Method
cpg	848.57	J/mol×K	858.37	Joback Method
cpg	862.91	J/mol×K	891.82	Joback Method
cpg	876.10	J/mol×K	925.27	Joback Method
cpg	888.17	J/mol×K	958.73	Joback Method
cpg	899.14	J/mol×K	992.18	Joback Method
cpg	909.02	J/mol×K	1025.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392688&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