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

Inchi: InChI=1S/C20H31NO5/c1-4-5-6-10-13-25-19(22)17(2)21(3)20(23)26-15-14-24-16-18-11-
InchiKey: XOXZBNVLJVABFX-UHFFFAOYSA-N
Formula: C20H31NO5
SMILES: CCCCCCOC(=O)C(C)N(C)C(=O)OCCOCc1ccccc1
Mol. weight [g/mol]: 365.46

Physical Properties

Property code	Value	Unit	Source
gf	-234.57	kJ/mol	Joback Method
hf	-779.17	kJ/mol	Joback Method
hfus	47.86	kJ/mol	Joback Method
hvap	84.77	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.784		Crippen Method
mcvol	299.630	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	2501.00		NIST Webbook
rinpol	2501.00		NIST Webbook
tb	870.68	K	Joback Method
tc	1073.15	K	Joback Method
tf	525.60	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.82	J/mol×K	870.68	Joback Method
cpg	966.65	J/mol×K	904.43	Joback Method
cpg	981.21	J/mol×K	938.17	Joback Method
cpg	994.55	J/mol×K	971.92	Joback Method
cpg	1006.68	J/mol×K	1005.66	Joback Method
cpg	1017.63	J/mol×K	1039.41	Joback Method
cpg	1027.42	J/mol×K	1073.15	Joback Method

Sources

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=U392690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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