

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

InChI: InChI=1S/C23H37NO5/c1-4-5-6-7-8-9-13-16-28-22(25)20(2)24(3)23(26)29-18-17-27-19-2
InChIKey: CAPJXHJKIHGXOQ-UHFFFAOYSA-N

Formula: C23H37NO5

SMILES: CCCCCCCCOC(=O)C(C)N(C)C(=O)OCCOCc1cccc1

Mol. weight [g/mol]: 407.54

Physical Properties

Property code	Value	Unit	Source
gf	-209.31	kJ/mol	Joback Method
hf	-841.09	kJ/mol	Joback Method
hfus	55.63	kJ/mol	Joback Method
hvap	91.44	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.954		Crippen Method
mcvol	341.900	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	2783.00		NIST Webbook
rinpol	2783.00		NIST Webbook
tb	939.32	K	Joback Method
tc	1150.41	K	Joback Method
tf	559.41	K	Joback Method
vc	1.294	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.26	J/mol×K	939.32	Joback Method
cpg	1148.58	J/mol×K	974.50	Joback Method
cpg	1163.45	J/mol×K	1009.68	Joback Method
cpg	1176.90	J/mol×K	1044.87	Joback Method
cpg	1188.97	J/mol×K	1080.05	Joback Method
cpg	1199.70	J/mol×K	1115.23	Joback Method
cpg	1209.12	J/mol×K	1150.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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