DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-hexyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C21H40N2O5/c1-7-9-11-13-15-27-20(25)18(4)22(5)19(24)17(3)23(6)21(26)28-
InchiKey: RUIXDRIGPPUQHE-UHFFFAOYSA-N
Formula: C21H40N2O5
SMILES: CCCCCCOC(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)OCCCCCC
Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-254.14	kJ/mol	Joback Method
hf	-954.45	kJ/mol	Joback Method
hfus	56.31	kJ/mol	Joback Method
hvap	90.71	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.994		Crippen Method
mcvol	343.160	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	910.33	K	Joback Method
tc	1114.54	K	Joback Method
tf	555.62	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.75	J/mol×K	910.33	Joback Method
cpg	1158.22	J/mol×K	944.36	Joback Method
cpg	1174.36	J/mol×K	978.40	Joback Method
cpg	1189.21	J/mol×K	1012.43	Joback Method
cpg	1202.81	J/mol×K	1046.47	Joback Method
cpg	1215.21	J/mol×K	1080.50	Joback Method
cpg	1226.44	J/mol×K	1114.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392648&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
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
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