DL-Alanyl-DL-alanyl-DL-alanine, N,N',N''-trimethyl-N'''-hexyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C25H47N3O6/c1-9-11-13-15-17-33-24(31)21(5)27(7)22(29)19(3)26(6)23(30)20
InchiKey: MXWYSIJQYICTQA-UHFFFAOYSA-N
Formula: C25H47N3O6
SMILES: CCCCCCOC(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)OCCCCCC
Mol. weight [g/mol]: 485.66

Physical Properties

Property code	Value	Unit	Source
gf	-241.04	kJ/mol	Joback Method
hf	-1087.34	kJ/mol	Joback Method
hfus	67.77	kJ/mol	Joback Method
hvap	108.01	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.841		Crippen Method
mcvol	411.070	ml/mol	McGowan Method
pc	874.28	kPa	Joback Method
rinpol	3009.00		NIST Webbook
rinpol	3009.00		NIST Webbook
tb	1067.72	K	Joback Method
tc	1325.01	K	Joback Method
tf	668.10	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1449.60	J/mol×K	1067.72	Joback Method
cpg	1466.89	J/mol×K	1110.60	Joback Method
cpg	1482.16	J/mol×K	1153.48	Joback Method
cpg	1495.53	J/mol×K	1196.36	Joback Method
cpg	1507.12	J/mol×K	1239.24	Joback Method
cpg	1517.04	J/mol×K	1282.12	Joback Method
cpg	1525.41	J/mol×K	1325.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392649&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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