DL-Alanyl-DL-alanyl-DL-alanine, N,N',N''-trimethyl-N''-(2-ethylhexyloxycarbonyl)-, 2-ethylhexyl ester

Inchi: InChI=1S/C29H55N3O6/c1-11-15-17-24(13-3)19-37-28(35)23(7)31(9)26(33)21(5)30(8)27(34)22(6)32(10)29(36)38-20-25(14-4)18-16-12-2/h21-25H,11-20H2,1-10H3

InchiKey: LNMUCUBIAKPLPK-UHFFFAOYSA-N

Formula: C29H55N3O6

SMILES: CCCCC(CC)COC(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 541.76

Physical Properties

Property code	Value	Unit	Source
gf	-212.24	kJ/mol	Joback Method
hf	-1180.46	kJ/mol	Joback Method
hfus	71.09	kJ/mol	Joback Method
hvap	116.14	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.113		Crippen Method
mcvol	467.430	ml/mol	McGowan Method
pc	711.11	kPa	Joback Method
rinpol	3230.00		NIST Webbook
rinpol	3230.00		NIST Webbook
tb	1158.36	K	Joback Method
tc	1467.55	K	Joback Method
tf	683.18	K	Joback Method
vc	1.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1702.54	J/mol×K	1158.36	Joback Method
cpg	1721.09	J/mol×K	1209.89	Joback Method
cpg	1736.83	J/mol×K	1261.42	Joback Method
cpg	1750.01	J/mol×K	1312.95	Joback Method
cpg	1760.85	J/mol×K	1364.49	Joback Method
cpg	1769.62	J/mol×K	1416.02	Joback Method
cpg	1776.56	J/mol×K	1467.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392672&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