DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-octyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C25H48N2O5/c1-7-9-11-13-15-17-19-31-24(29)22(4)26(5)23(28)21(3)27(6)25(

InchiKey: GNYLFSFQRJKHMR-UHFFFAOYSA-N

Formula: C25H48N2O5

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

Mol. weight [g/mol]: 456.66

Physical Properties

Property code	Value	Unit	Source
gf	-220.46	kJ/mol	Joback Method
hf	-1037.01	kJ/mol	Joback Method
hfus	66.67	kJ/mol	Joback Method
hvap	99.61	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.554		Crippen Method
mcvol	399.520	ml/mol	McGowan Method
pc	839.67	kPa	Joback Method
rinpol	2872.00		NIST Webbook
rinpol	2872.00		NIST Webbook
tb	1001.85	K	Joback Method
tc	1236.45	K	Joback Method
tf	600.70	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1391.25	J/mol×K	1001.85	Joback Method
cpg	1410.52	J/mol×K	1040.95	Joback Method
cpg	1427.97	J/mol×K	1080.05	Joback Method
cpg	1443.70	J/mol×K	1119.15	Joback Method
cpg	1457.77	J/mol×K	1158.25	Joback Method
cpg	1470.28	J/mol×K	1197.35	Joback Method
cpg	1481.29	J/mol×K	1236.45	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=U392657&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

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