

DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-(2-ethylhexyloxycarbonyl)-, 2-ethylhexylester

InChI: InChI=1S/C25H48N2O5/c1-9-13-15-21(11-3)17-31-24(29)20(6)26(7)23(28)19(5)27(8)25(2,4)/N

InChIKey: CDKSCVAOBIRQRM-UHFFFAOYSA-N

Formula: C25H48N2O5

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

Mol. weight [g/mol]: 456.66

Physical Properties

Property code	Value	Unit	Source
gf	-225.34	kJ/mol	Joback Method
hf	-1047.57	kJ/mol	Joback Method
hfus	59.63	kJ/mol	Joback Method
hvap	98.84	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.266		Crippen Method
mvol	399.520	ml/mol	McGowan Method
pc	847.51	kPa	Joback Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook
tb	1000.97	K	Joback Method
tc	1232.10	K	Joback Method
tf	570.70	K	Joback Method
vc	1.502	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1391.87	J/molxK	1000.97	Joback Method
cpg	1410.74	J/molxK	1039.49	Joback Method
cpg	1427.82	J/molxK	1078.01	Joback Method
cpg	1443.18	J/molxK	1116.53	Joback Method
cpg	1456.92	J/molxK	1155.06	Joback Method
cpg	1469.09	J/molxK	1193.58	Joback Method
cpg	1479.78	J/molxK	1232.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392671&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
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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