DL-3-Aminobutanoic acid, N-(2-ethylhexyl)oxycarbonyl-, 2-ethylhexyl ester

Inchi: InChI=1S/C21H41NO4/c1-6-10-12-18(8-3)15-25-20(23)14-17(5)22-21(24)26-16-19(9-4)1

InchiKey: URVNUTJHEVPINU-UHFFFAOYSA-N

Formula: C21H41NO4

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

Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
hf	-949.43	kJ/mol	Joback Method
hvap	92.81	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.672		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	983.31	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	946.01	K	Joback Method
tc	1159.29	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392829&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

hf: Enthalpy of formation 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