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

Inchi: InChI=1S/C23H45NO4/c1-5-8-10-11-12-13-14-15-17-27-22(25)18-20(4)24-23(26)28-19-2

InchiKey: XRLZGHANDQIALO-UHFFFAOYSA-N

Formula: C23H45NO4

SMILES: CCCCCCCCCCOC(=O)CC(C)N=C(O)OCC(CC)CCCC

Mol. weight [g/mol]: 399.61

Physical Properties

Property code	Value	Unit	Source
hf	-985.43	kJ/mol	Joback Method
hvap	97.65	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	6.596		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
pc	870.68	kPa	Joback Method
rinpol	2683.00		NIST Webbook
rinpol	2683.00		NIST Webbook
tb	992.21	K	Joback Method
tc	1222.74	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392822&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

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