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

Inchi: InChI=1S/C19H37NO4/c1-5-8-10-11-13-23-18(21)14-16(4)20-19(22)24-15-17(7-3)12-9-6

InchiKey: JFQJIIMFHDYDST-UHFFFAOYSA-N

Formula: C19H37NO4

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

Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
hf	-902.87	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	5.036		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	900.69	K	Joback Method
tc	1102.71	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392819&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