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

Inchi: InChI=1S/C22H43NO4/c1-5-8-10-11-12-13-14-16-26-21(24)17-19(4)23-22(25)27-18-20(

InchiKey: FWTFTZXWGAAKKP-UHFFFAOYSA-N

Formula: C22H43NO4

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

Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
hf	-964.79	kJ/mol	Joback Method
hvap	95.43	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.206		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	922.18	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	969.33	K	Joback Method
tc	1191.02	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392821&Units=SI

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