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

Inchi: InChI=1S/C28H55NO4/c1-5-8-10-11-12-13-14-15-16-17-18-19-20-22-32-27(30)23-25(4)2

InchiKey: WKIGYRSFZYBHDZ-UHFFFAOYSA-N

Formula: C28H55NO4

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

Mol. weight [g/mol]: 469.74

Physical Properties

Property code	Value	Unit	Source
hf	-1088.63	kJ/mol	Joback Method
hvap	108.78	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	8.546		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
pc	668.04	kPa	Joback Method
rinpol	3174.00		NIST Webbook
rinpol	3174.00		NIST Webbook
tb	1106.61	K	Joback Method
tc	1403.05	K	Joback Method

Sources

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=U392827&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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