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

Inchi: InChI=1S/C27H53NO4/c1-5-8-10-11-12-13-14-15-16-17-18-19-21-31-26(29)22-24(4)28-2
InchiKey: ZNKZIYKTUFHMLI-UHFFFAOYSA-N
Formula: C27H53NO4
SMILES: CCCCCCCCCCCCCCOC(=O)CC(C)N=C(O)OCC(CC)CCCC
Mol. weight [g/mol]: 455.71

Physical Properties

Property code	Value	Unit	Source
hf	-1067.99	kJ/mol	Joback Method
hvap	106.56	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	8.156		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	702.47	kPa	Joback Method
rinpol	3069.00		NIST Webbook
rinpol	3069.00		NIST Webbook
tb	1083.73	K	Joback Method
tc	1363.71	K	Joback Method

Sources

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=U392826&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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