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

Inchi: InChI=1S/C24H47NO4/c1-5-8-10-11-12-13-14-15-16-18-28-23(26)19-21(4)25-24(27)29-2
InchiKey: AKGHEMYFECZURY-UHFFFAOYSA-N
Formula: C24H47NO4
SMILES: CCCCCCCCCCCOC(=O)CC(C)N=C(O)OCC(CC)CCCC
Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
hf	-1006.07	kJ/mol	Joback Method
hvap	99.88	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.986		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	823.37	kPa	Joback Method
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	1015.09	K	Joback Method
tc	1255.77	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392823&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