2-Aminopent-4-enoic acid, N-(2-ethylhexyloxycarbonyl)-, tetradecyl ester

Inchi: InChI=1S/C28H53NO4/c1-5-9-11-12-13-14-15-16-17-18-19-20-23-32-27(30)26(21-7-3)29

InchiKey: HGJAZJWOCPTHDY-UHFFFAOYSA-N

Formula: C28H53NO4

SMILES: C=CCC(N=C(O)OCC(CC)CCCC)C(=O)OCCCCCCCCCCCCCC

Mol. weight [g/mol]: 467.72

Physical Properties

Property code	Value	Unit	Source
hf	-963.20	kJ/mol	Joback Method
hvap	108.11	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	8.322		Crippen Method
mcvol	425.940	ml/mol	McGowan Method
pc	682.78	kPa	Joback Method
tb	1103.29	K	Joback Method
tc	1393.77	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393169&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature