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

Inchi: InChI=1S/C25H47NO4/c1-5-9-11-12-13-14-15-16-17-20-29-24(27)23(18-7-3)26-25(28)30

InchiKey: ILSSPMOEAQIIEZ-UHFFFAOYSA-N

Formula: C25H47NO4

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

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
hf	-901.28	kJ/mol	Joback Method
hvap	101.44	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	7.152		Crippen Method
mcvol	383.670	ml/mol	McGowan Method
pc	798.43	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	1034.65	K	Joback Method
tc	1283.08	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393166&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