2-Aminopent-4-enoic acid, N-hexyloxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C27H51NO4/c1-4-7-9-11-12-13-14-15-16-17-18-19-21-23-31-26(29)25(22-6-3)

InchiKey: AESKWOMNJVGSGV-UHFFFAOYSA-N

Formula: C27H51NO4

SMILES: C=CCC(N=C(O)OCCCCCC)C(=O)OCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
hf	-937.28	kJ/mol	Joback Method
hvap	106.28	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	8.076		Crippen Method
mcvol	411.850	ml/mol	McGowan Method
pc	715.30	kPa	Joback Method
rinpol	3033.00		NIST Webbook
rinpol	3033.00		NIST Webbook
tb	1080.85	K	Joback Method
tc	1359.32	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=U393148&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