1-Aminocyclopentanecarboxylic acid, N-(but-3-en-1-yloxycarbonyl)-, tridecyl ester

Inchi: InChI=1S/C24H43NO4/c1-3-5-7-8-9-10-11-12-13-14-17-21-28-22(26)24(18-15-16-19-24)

InchiKey: PKNHIKSPLJTSGV-UHFFFAOYSA-N

Formula: C24H43NO4

SMILES: C=CCCOC(O)=NC1(C(=O)OCCCCCCCCCCCCCC)CCCC1

Mol. weight [g/mol]: 409.60

Physical Properties

Property code	Value	Unit	Source
hf	-794.36	kJ/mol	Joback Method
hvap	99.09	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.660		Crippen Method
mcvol	358.720	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	1028.17	K	Joback Method
tc	1262.26	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392601&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