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

Inchi: InChI=1S/C27H49NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-20-24-31-25(29)27(21-18-
InchiKey: CHTYJYSQZSLBFK-UHFFFAOYSA-N
Formula: C27H49NO4
SMILES: C=CCCOC(O)=NC1(C(=O)OCCCCCCCCCCCCCCCC)CCCC1
Mol. weight [g/mol]: 451.68

Physical Properties

Property code	Value	Unit	Source
hf	-856.28	kJ/mol	Joback Method
hvap	105.77	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.830		Crippen Method
mcvol	400.990	ml/mol	McGowan Method
pc	806.16	kPa	Joback Method
rinpol	3059.00		NIST Webbook
tb	1096.81	K	Joback Method
tc	1360.89	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392604&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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