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

Inchi: InChI=1S/C26H47NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-19-23-30-24(28)26(20-17-18-
InchiKey: IYIITGXHCFSEFG-UHFFFAOYSA-N
Formula: C26H47NO4
SMILES: C=CCCOC(O)=NC1(C(=O)OCCCCCCCCCCCCCCC)CCCC1
Mol. weight [g/mol]: 437.66

Physical Properties

Property code	Value	Unit	Source
hf	-835.64	kJ/mol	Joback Method
hvap	103.54	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.440		Crippen Method
mcvol	386.900	ml/mol	McGowan Method
pc	851.97	kPa	Joback Method
rinpol	2955.00		NIST Webbook
tb	1073.93	K	Joback Method
tc	1326.61	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392603&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