1-Aminocyclopentanecarboxylic acid, N-((1R)-(-)-menthyloxycarbonyl)-, tridecyl ester

Inchi: InChI=1S/C30H55NO4/c1-5-6-7-8-9-10-11-12-13-14-17-22-34-28(32)30(20-15-16-21-30)31-29(33)35-26-23-25(4)19-18-24(3)27(26)2/h24-27H,5-23H2,1-4H3,(H,31,33)/t24-,25-,26+,27+/m1/s1

InchiKey: OLTWZNDKUTWSHA-UHFFFAOYSA-N

Formula: C30H55NO4

SMILES: CCCCCCCCCCCCCOC(=O)C1(N=C(O)OC2CC(C)CCC2C(C)C)CCCC1

Mol. weight [g/mol]: 493.76

Physical Properties

Property code	Value	Unit	Source
hf	-1035.27	kJ/mol	Joback Method
hvap	112.54	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.545		Crippen Method
mcvol	436.700	ml/mol	McGowan Method
pc	728.49	kPa	Joback Method
rinpol	3227.00		NIST Webbook
tb	1178.54	K	Joback Method
tc	1464.88	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392620&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