1-Aminocyclopentanecarboxylic acid, N-(propoxycarbonyl)-, tridecyl ester

Inchi: InChI=1S/C23H43NO4/c1-3-5-6-7-8-9-10-11-12-13-16-20-27-21(25)23(17-14-15-18-23)2

InchiKey: HRPKMILPONGLJD-UHFFFAOYSA-N

Formula: C23H43NO4

SMILES: CCCCCCCCCCCCCOC(=O)C1(N=C(O)OCCC)CCCC1

Mol. weight [g/mol]: 397.59

Physical Properties

Property code	Value	Unit	Source
hf	-899.15	kJ/mol	Joback Method
hvap	97.54	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.494		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2768.00		NIST Webbook
tb	1008.61	K	Joback Method
tc	1236.94	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392497&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