1-Aminocyclopentanecarboxylic acid, 3-chloropropoxycarbonyl-, tridecyl ester

Inchi: InChI=1S/C23H42ClNO4/c1-2-3-4-5-6-7-8-9-10-11-14-19-28-21(26)23(16-12-13-17-23)2

InchiKey: MHCNBCWVFFUGLH-UHFFFAOYSA-N

Formula: C23H42ClNO4

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

Mol. weight [g/mol]: 432.04

Physical Properties

Property code	Value	Unit	Source
hf	-914.89	kJ/mol	Joback Method
hvap	101.92	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.713		Crippen Method
mcvol	361.170	ml/mol	McGowan Method
pc	966.27	kPa	Joback Method
tb	1046.04	K	Joback Method
tc	1285.02	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392630&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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