1-Aminocyclopentanecarboxylic acid, N-(2-chloroethoxycarbonyl)-, propyl ester

Inchi: InChI=1S/C12H20ClNO4/c1-2-8-17-10(15)12(5-3-4-6-12)14-11(16)18-9-7-13/h2-9H2,1H3

InchiKey: GUYPNUZOKUGBQL-UHFFFAOYSA-N

Formula: C12H20ClNO4

SMILES: CCCOC(=O)C1(N=C(O)OCCCl)CCCC1

Mol. weight [g/mol]: 277.75

Physical Properties

Property code	Value	Unit	Source
hf	-687.85	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.422		Crippen Method
mcvol	206.180	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	794.36	K	Joback Method
tc	1002.07	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392548&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