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

Inchi: InChI=1S/C13H21Cl2NO4/c14-7-3-9-19-11(17)13(5-1-2-6-13)16-12(18)20-10-4-8-15/h1-
InchiKey: VACHLNLIUUKJEF-UHFFFAOYSA-N
Formula: C13H21Cl2NO4
SMILES: O=C(OCCCCl)C1(N=C(O)OCCCCl)CCCC1
Mol. weight [g/mol]: 326.22

Physical Properties

Property code	Value	Unit	Source
hf	-724.23	kJ/mol	Joback Method
hvap	84.05	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	3.031		Crippen Method
mcvol	232.510	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	2265.00		NIST Webbook
rinpol	2265.00		NIST Webbook
tb	854.67	K	Joback Method
tc	1065.45	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392631&Units=SI

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