Glycine, 2-cyclohexyl-N-(3-chloropropoxycarbonyl)-, octyl ester

Inchi: InChI=1S/C20H36ClNO4/c1-2-3-4-5-6-10-15-25-19(23)18(17-12-8-7-9-13-17)22-20(24)2

InchiKey: GLILSDAECHOUDG-UHFFFAOYSA-N

Formula: C20H36ClNO4

SMILES: CCCCCCCCOC(=O)C(N=C(O)OCCCCl)C1CCCCC1

Mol. weight [g/mol]: 389.96

Physical Properties

Property code	Value	Unit	Source
hf	-879.65	kJ/mol	Joback Method
hvap	96.18	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.399		Crippen Method
mcvol	318.900	ml/mol	McGowan Method
pc	1156.14	kPa	Joback Method
rinpol	2676.00		NIST Webbook
rinpol	2676.00		NIST Webbook
tb	980.99	K	Joback Method
tc	1201.09	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=U392339&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature