Cyclohexanecarboxylic acid, 1-[3-(2-chloroethyl)ureido]-3-methyl-, ethyl ester

Inchi: InChI=1S/C13H23ClN2O3/c1-3-19-11(17)13(6-4-5-10(2)9-13)16-12(18)15-8-7-14/h10H,3

InchiKey: XCXXHYFJPSOAQX-UHFFFAOYSA-N

Formula: C13H23ClN2O3

SMILES: CCOC(=O)C1(NC(O)=NCCCl)CCCC(C)C1

Mol. weight [g/mol]: 290.79

CAS: 33190-16-8

Physical Properties

Property code	Value	Unit	Source
hf	-549.30	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.241		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
tb	844.59	K	Joback Method
tc	1057.65	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33190168&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature