Cyclopentanecarboxylic aicd, 1-[3-(2-chloroethyl)-3-nitrosoureido]-, ethyl ester

Inchi: InChI=1S/C11H18ClN3O4/c1-2-19-9(16)11(5-3-4-6-11)13-10(17)15(14-18)8-7-12/h2-8H2

InchiKey: DQKFATBSGXKDEH-UHFFFAOYSA-N

Formula: C11H18ClN3O4

SMILES: CCOC(=O)C1(NC(=O)N(CCCl)N=O)CCCC1

Mol. weight [g/mol]: 291.73

CAS: 13909-05-2

Physical Properties

Property code	Value	Unit	Source
hf	-614.96	kJ/mol	Joback Method
hvap	77.05	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	1.794		Crippen Method
mcvol	207.750	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	760.20	K	Joback Method
tc	968.26	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13909052&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