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

Inchi: InChI=1S/C12H20ClN3O4/c1-2-20-10(17)12(6-4-3-5-7-12)14-11(18)16(15-19)9-8-13/h2-9

InchiKey: FPIQZBQZKBKLEI-UHFFFAOYSA-N

Formula: C12H20ClN3O4

SMILES: CCOC(=O)C1(NC(=O)N(CCCl)N=O)CCCCC1

Mol. weight [g/mol]: 305.76

CAS: 13991-74-7

Physical Properties

Property code	Value	Unit	Source
hf	-641.76	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.184		Crippen Method
mcvol	221.840	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
tb	787.35	K	Joback Method
tc	998.44	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13991747&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