[4-(([1-(2-Chloroethyl)-2-oxohydrazino]carbonyl)a
acid

Inchi: InChI=1S/C11H12ClN3O4/c12-5-6-15(14-19)11(18)13-9-3-1-8(2-4-9)7-10(16)17/h1-4H,5
InchiKey: ISHRKCISRZYJGC-UHFFFAOYSA-N
Formula: C11H12ClN3O4
SMILES: O=NN(CCCl)C(=O)Nc1ccc(CC(=O)O)cc1
Mol. weight [g/mol]: 285.68
CAS: 13909-29-0

Physical Properties

Property code	Value	Unit	Source
hf	-485.63	kJ/mol	Joback Method
hvap	95.15	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.068		Crippen Method
mcvol	194.850	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
tb	846.10	K	Joback Method
tc	1053.70	K	Joback Method

Sources

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=C13909290&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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