

[4-(([1-(2-Chloroethyl)-2-oxohydrazino]carbonyl)amino)acetic 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,5-6H2
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C13909290&Units=SI

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

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