Acetic acid, [p-[3-(2-chloroethyl)-3-nitrosoureido]phenylthio]-

Inchi: InChI=1S/C11H12ClN3O4S/c12-5-6-15(14-19)11(18)13-8-1-3-9(4-2-8)20-7-10(16)17/h1-

InchiKey: HDWAURNNJRJXQP-UHFFFAOYSA-N

Formula: C11H12ClN3O4S

SMILES: O=NN(CCCl)C(=O)Nc1ccc(SCC(=O)O)cc1

Mol. weight [g/mol]: 317.75

CAS: 13909-30-3

Physical Properties

Property code	Value	Unit	Source
hf	-443.76	kJ/mol	Joback Method
hvap	101.97	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.617		Crippen Method
mcvol	211.200	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	914.88	K	Joback Method
tc	1135.60	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13909303&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

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