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

Inchi: InChI=1S/C10H10ClN3O4/c11-5-6-14(13-18)10(17)12-8-3-1-7(2-4-8)9(15)16/h1-4H,5-6H

InchiKey: XXPHTAWBJVUIOY-UHFFFAOYSA-N

Formula: C10H10ClN3O4

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

Mol. weight [g/mol]: 271.66

CAS: 13909-25-6

Physical Properties

Property code	Value	Unit	Source
hf	-464.99	kJ/mol	Joback Method
hvap	92.92	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.139		Crippen Method
mcvol	180.760	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	823.22	K	Joback Method
tc	1031.38	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=C13909256&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