Benzoic acid, 3,5-bis[3-(2-chloroethyl)-3-nitrosoureido]-

Inchi: InChI=1S/C13H14Cl2N6O6/c14-1-3-20(18-26)12(24)16-9-5-8(11(22)23)6-10(7-9)17-13(2

InchiKey: RRTCCTJFLQKSPL-UHFFFAOYSA-N

Formula: C13H14Cl2N6O6

SMILES: O=NN(CCCl)C(O)=Nc1cc(N=C(O)N(CCCl)N=O)cc(C(=O)O)c1

Mol. weight [g/mol]: 421.19

CAS: 13907-61-4

Physical Properties

Property code	Value	Unit	Source
hf	-755.27	kJ/mol	Joback Method
hvap	142.75	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.920		Crippen Method
mcvol	268.350	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	1243.55	K	Joback Method
tc	1554.47	K	Joback Method

Sources

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=C13907614&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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