Benzoic acid, 4-[3-(2-chloroethyl)-3-nitrosoureido]-3,5-dimethyl-

Inchi: InChI=1S/C12H14ClN3O4/c1-7-5-9(11(17)18)6-8(2)10(7)14-12(19)16(15-20)4-3-13/h5-6

InchiKey: JCVIOXBESVVEDT-UHFFFAOYSA-N

Formula: C12H14ClN3O4

SMILES: Cc1cc(C(=O)O)cc(C)c1NC(=O)N(CCCl)N=O

Mol. weight [g/mol]: 299.71

CAS: 116465-95-3

Physical Properties

Property code	Value	Unit	Source
hf	-529.21	kJ/mol	Joback Method
hvap	98.70	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	2.756		Crippen Method
mcvol	208.940	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	878.94	K	Joback Method
tc	1088.37	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=C116465953&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