Benzamide, 5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxy-

Other names:

2',5-Dichlor-4'-nitro-salizylsaeureanilid
2',5-Dichloro-4'-Nitrosalicylanilide
2-Chloro-4-nitrophenylamide-6-chlorosalicylic acid
2-Hydroxy-5-chloro-N-(2-chloro-4-nitrophenyl)benzamide
5-Chloro-2'-chloro-4'-nitrosalicylanilide
5-Chloro-N-(2'-chloro-4'-nitrophenyl)salicylamide
5-Chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxybenzamide (niclosamide)
5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxybenzamide
Atenase
BAY 2353
Bayer 2353
Bayer 73
Bayluscid
Cestocid
Cestocide
Chemagro 2353
Devermin
Devermine
Dichlosale
ENT 25823
Fedal-Telmin
Fenasal
HL 2447
Helmiantin
Iomesan
Iomezan
Lintex
Mansonil
Mato
N-(2'-Chlor-4'-nitrophenyl)-5-chlorsalicylamid
N-(2'-Chloro-4'-nitrophenyl)-5-chlorosalicylamide
N-(2-Chloro-4-nitrophenyl)-5-chlorosalicylamide
Nasemo
Niclocide
Phenasal
Radeverm
Ruby
Sagimid
Salicylanilide, 2',5-dichloro-4'-nitro-
Sulqui

	Tredemine
	Vermitid
	Vermitin
	WR 46234
	Yomesan
	Zestocarp
	niclosamide
Inchi:	InChI=1S/C13H8Cl2N2O4/c14-7-1-4-12(18)9(5-7)13(19)16-11-3-2-8(17(20)21)6-10(11)1
InchiKey:	RJMUSRYZPJIFPJ-UHFFFAOYSA-N
Formula:	C13H8Cl2N2O4
SMILES:	O=C(Nc1ccc([N+](=O)[O-])cc1Cl)c1cc(Cl)ccc1O
Mol. weight [g/mol]:	327.12

Physical Properties

Property code	Value	Unit	Source
hf	-233.54	kJ/mol	Cheméo Relay (1.0)
hfus	48.58	kJ/mol	Joback Method
hvap	124.01	kJ/mol	Cheméo Relay (1.0)
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-4.70		Aqueous Solubility Prediction Method
log10ws	-4.70		Estimated Solubility Method
logp	3.859		Crippen Method
mcvol	205.830	ml/mol	McGowan Method
tb	636.68	K	Cheméo Relay (1.0)
tf	499.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.33	J/mol×K	976.50	Joback Method
cpg	559.25	J/mol×K	1022.35	Joback Method
cpg	567.95	J/mol×K	1068.20	Joback Method
cpg	576.59	J/mol×K	1114.04	Joback Method
cpg	585.34	J/mol×K	1159.89	Joback Method
cpg	594.37	J/mol×K	1205.74	Joback Method

cpg	603.85	J/mol×K	1251.59	Joback Method
hfust	40.70	kJ/mol	505.40	NIST Webbook
hfust	35.98	kJ/mol	502.20	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Cheméo Relay (1.0):

Phase solubility studies of poorly soluble drug molecules by using O-phosphorylated calixarenes as drug solubilizing agents: https://www.doi.org/10.1021/je200992c

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50657&Units=SI

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

Cheméo Relay (1.0, beta):

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point