Niclosamide

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
5-Chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxybenzamide (niclosamide)
Atenase
BAY 2353
Bayer 2353
Bayer 73
Bayluscid
Benzamide, 5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxy-
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

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

CAS: 50-65-7

Physical Properties

Property code	Value	Unit	Source
gf	72.05	kJ/mol	Joback Method
hf	-151.66	kJ/mol	Joback Method
hfus	48.58	kJ/mol	Joback Method
hvap	102.63	kJ/mol	Joback Method
log10ws	-4.70		Estimated Solubility Method
log10ws	-4.70		Aqueous Solubility Prediction Method
logp	3.859		Crippen Method
mcvol	205.830	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	976.50	K	Joback Method
tc	1251.59	K	Joback Method
tf	499.65	K	Aqueous Solubility Prediction Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.34	J/mol×K	1159.89	Joback Method
cpg	594.37	J/mol×K	1205.74	Joback Method

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	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

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

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

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

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

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

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

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
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
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
tf: Normal melting (fusion) point
vc: Critical Volume