Chlorthalidone

Other names:	(.+/-.)-Chlorthalidone
	(.+/-.)-Hygroton
	1-Keto-3-(3'-sulfamyl-4'-chlorophenyl)-3-hydroxyisoindoline
	1-Oxo-3-(3-sulfamyl-4-chlorophenyl)-3-hydroxyisoindoline
	2-Chloro-5-(1-hydroxy-3-oxo-1-isoindolinyl)benzenesulfonamide
	2-Chloro-5-(1-hydroxy-3-oxo-1H-isoindolinyl)benzenesulfonamide
	3-(4'-Chloro-3'-sulfamoylphenyl)-3-hydroxyphthalimidine
	3-Hydroxy-3-(4-chloro-3-sulfamylphenyl)phthalimidine
	Benzenesulfonamide, 2-chloro-5-(1-hydroxy-3-oxo-1-isoindolinyl)-
	Benzenesulfonamide, 2-chloro-5-(2,3-dihydro-1-hydroxy-3-oxo-1H-isoindol-1-yl)-
	Chlorothalidone
	Chlorphthalidolone
	Chlorphthalidone
	Chlortalidone
	Chlorthalidon
	Demi-regroton
	G 33182
	Hydro-Long
	Hygroton
	Igroton
	Isoren
	NSC-69200
	Natriuran
	Oksodolin
	Oradil
	Oxodolin
	Phthalamodine
	Phthalamudine
	Racemic chlorthalidone
	Renon
	Saluretin
	Tenoretic
	Thalitone
	Zambesil
Inchi:	InChI=1S/C14H11ClN2O4S/c15-11-6-5-8(7-12(11)22(16,20)21)14(19)10-4-2-1-3-9(10)13
InchiKey:	JIVPVXMEBJLZRO-UHFFFAOYSA-N
Formula:	C14H11ClN2O4S
SMILES:	NS(=O)(=O)c1cc(C2(O)NC(=O)c3ccccc32)ccc1Cl
Mol. weight [g/mol]:	338.77
CAS:	77-36-1

Physical Properties

Property code	Value	Unit	Source
gf	-267.53	kJ/mol	Joback Method
hf	-493.02	kJ/mol	Joback Method
hfus	44.73	kJ/mol	Joback Method
hvap	113.40	kJ/mol	Joback Method
log10ws	-3.45		Estimated Solubility Method
log10ws	-3.45		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-3.39		Aqueous Solubility Prediction Method
logp	0.924		Crippen Method
mcvol	217.470	ml/mol	McGowan Method
pc	4802.50	kPa	Joback Method
tb	961.29	K	Joback Method
tc	1214.28	K	Joback Method
tf	765.59	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.62	J/mol×K	961.29	Joback Method
cpg	646.00	J/mol×K	1003.46	Joback Method
cpg	658.30	J/mol×K	1045.62	Joback Method
cpg	670.67	J/mol×K	1087.79	Joback Method
cpg	683.28	J/mol×K	1129.95	Joback Method
cpg	696.28	J/mol×K	1172.12	Joback Method
cpg	709.82	J/mol×K	1214.28	Joback Method

Sources

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
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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