Chlorothiazide

Other names:	2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-, 1,1-dioxide
	6-Chloro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
	6-Chloro-7-sulfamoyl-2H-1,2,4-benzothiadiazine 1,1-dioxide
	Alurene
	Chloriazid
	Chlorosal
	Chlorothiazid
	Chlorthiazide
	Chlortiazid
	Chlorurit
	Chlotride
	Chlrosal
	Clotride
	Diuresal
	Diuril
	Diuril Boluses
	Diurilix
	Diurite
	Diutrid
	Flumen
	Minzil
	NSC 25693
	Neo-Dema
	SK-chlorothiazide
	Salisan
	Salunil
	Saluretil
	Saluric
	Thiazide
	Urinex
	Warduzide
	Yadalan
Inchi:	InChI=1S/C7H6ClN3O4S2/c8-4-1-5-7(2-6(4)16(9,12)13)17(14,15)11-3-10-5/h1-3H,(H,10
InchiKey:	JBMKAUGHUNFTOL-UHFFFAOYSA-N
Formula:	C7H6ClN3O4S2
SMILES:	NS(=O)(=O)c1cc2c(cc1Cl)N=CNS2(=O)=O
Mol. weight [g/mol]:	295.72
CAS:	58-94-6

Physical Properties

Property code	Value	Unit	Source
gf	-493.43	kJ/mol	Joback Method
hf	-617.41	kJ/mol	Joback Method
hfus	49.35	kJ/mol	Joback Method
hvap	100.38	kJ/mol	Joback Method
log10ws	-3.05		Estimated Solubility Method
log10ws	-3.05		Aqueous Solubility Prediction Method
logp	-0.061		Crippen Method
mcvol	168.930	ml/mol	McGowan Method
pc	9122.35	kPa	Joback Method
tb	702.84	K	Joback Method
tc	947.15	K	Joback Method
tf	667.97	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.67	J/mol×K	702.84	Joback Method
cpg	424.37	J/mol×K	743.56	Joback Method
cpg	433.92	J/mol×K	784.28	Joback Method
cpg	442.30	J/mol×K	824.99	Joback Method
cpg	449.50	J/mol×K	865.71	Joback Method
cpg	455.51	J/mol×K	906.43	Joback Method
cpg	460.30	J/mol×K	947.15	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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58946&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