Hydrochlorothiazide

Other names:

2H-1,2,4-Benzothiadiazine, 6-chloro-3,4-dihydro-7-sulfamoyl-2, 1,1-dioxide
2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3,4-dihydro-, 1,1-dioxide
3,4-Dihydro-6-chloro-7-sulfamyl-1,2,4-benzothiadiazine-1,1-dioxide
3,4-Dihydrochlorothiazide
6-Chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
6-Chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide-1,1-dioxide (hydrochlorthiazide)
6-Chloro-3,4-dihydro-7-sulfamoyl-2H-1,2,4-benzothiadiazine 1,1-dioxide
6-Chloro-7-sulfamoyl-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide
6-Chloro-7-sulfamoyl-3,4-dihydrobenzo-1,2,4-thiadiazine-1,1-dioxide
6-Chloro-7-sulfamyl-3,4-dihydro-1,2,4-benzothiadiazine-1,1-dioxide
6-chloro-3,4-dihydro-2H-benzo[e][1,2,4]thiadiazine-7-sulfonamide 1,1-dioxide
Acuretic
Apresazide
Aquarills
Aquarius
Aquazide
Bremil
Caplaril
Carozide
Chlorosulthiadil
Chlorsulfonamidodihydrobenzothiadiazine dioxide
Chlorzide
Cidrex
Dichlorosal
Dichlotiazid
Dichlotride
Diclotride
Dihydrochlorothiazid
Dihydrochlorothiazide
Dihydrochlorothiazidum
Dihydrochlorurit
Dihydrochlorurite
Direma
Disalunil
Drenol
Dyazide
Esidrex
Esidrix
Fluvin
H-1,2,4-benzothiadiazine, 6-chloro-3,4-dihydro-7-sulfamoyl-2, 1,1-dioxide

H.H. 25/25
H.H. 50/50
HCTZ
HCZ
Hidril
Hidrochlortiazid
Hidroronol
Hidrotiazida
Hydril
Hydro-Aquil
Hydro-Diuril
Hydrochlorothiazid
Hydrochlorthiazide
Hydrochlorzide
Hydrocot
Hydrodiuretic
Hydrosaluric
Hydrothide
Hydrozide
Hypothiazid
Hypothiazide
Idrodiuvis
Idrotiazide
Ivaugan
Jen-Diril
Lopressor HCT
Lotensin HCT
Manschitt
Maschitt
Megadiuril
Microzide
Moduretic
NCI-C55925
Nefrix
Neo-codema
Neoflumen
Newtolide
Oretic
Panurin
Ro-hydrazide
Servithiazid
Su 5879
Thiaretic

Thiazide, hydrochloro-
Thiuretic
Thlaretic
Timolide
Unipres
Urirex
Urodiazin
Vaseretic
Vetidrex
Ziac
Zide

Inchi: InChI=1S/C7H8ClN3O4S2/c8-4-1-5-7(2-6(4)16(9,12)13)17(14,15)11-3-10-5/h1-2,10-11H

InchiKey: JZUFKLXOESDKRF-UHFFFAOYSA-N

Formula: C7H8ClN3O4S2

SMILES: NS(=O)(=O)c1cc2c(cc1Cl)NCNS2(=O)=O

Mol. weight [g/mol]: 297.74

CAS: 58-93-5

Physical Properties

Property code	Value	Unit	Source
gf	-552.46	kJ/mol	Joback Method
hf	-708.35	kJ/mol	Joback Method
hfus	52.58	kJ/mol	Joback Method
hvap	100.64	kJ/mol	Joback Method
log10ws	-2.63		Estimated Solubility Method
log10ws	-2.69		Aqueous Solubility Prediction Method
log10ws	-2.68		Aqueous Solubility Prediction Method
logp	-0.351		Crippen Method
mcvol	173.230	ml/mol	McGowan Method
pc	8916.78	kPa	Joback Method
tb	698.53	K	Joback Method
tc	937.04	K	Joback Method
tf	544.40	K	Aqueous Solubility Prediction Method
tf	544.40	K	Aqueous Solubility Prediction Method

tt	544.91	K	Measurement and Correlation of Solubility of Hydrochlorothiazide in Monosolvents and Binary Solvent Mixtures from 283.15 to 323.15 K
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.14	J/mol×K	857.54	Joback Method
cpg	459.90	J/mol×K	897.29	Joback Method
cpg	415.86	J/mol×K	698.53	Joback Method
cpg	426.70	J/mol×K	738.28	Joback Method
cpg	436.54	J/mol×K	778.03	Joback Method
cpg	445.35	J/mol×K	817.79	Joback Method
cpg	465.63	J/mol×K	937.04	Joback Method
hfust	33.60	kJ/mol	540.80	NIST Webbook
hfust	30.96	kJ/mol	547.20	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/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=C58935&Units=SI

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

Measurement and Correlation of Solubility of Hydrochlorothiazide in Monosolvents and Binary Solvent Mixtures from 283.15 to 323.15 K: https://www.doi.org/10.1021/acs.jced.9b00220

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

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

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
tt:	Triple Point Temperature
vc:	Critical Volume