

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
(hydrochlorothiazide)
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
Flavin
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

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|-----------------------------|--|
| Inchi: | InChI=1S/C7H8CIN3O4S2/c8-4-1-5-7(2-6(4)16(9,12)13)17(14,15)11-3-10-5/h1-2,10-11H |
| InchiKey: | JZUFLXOESDKRF-UHFFFAOYSA-N |
| Formula: | C7H8CIN3O4S2 |
| 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 |

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|----|--------|---------|--|
| 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/AqueousDataset003.xlsx |
| 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/ci9903071 |
| 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 |
| Aqueous Solubility Prediction Method: | https://en.wikipedia.org/wiki/Joback_method |
| | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx |

Legend

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|------|--|
| 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 |

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