# Benzthiazide

**Other names:**

2H-1,2,4-Benzothiadiazine-7-sulfonamide, 3-((benzylthio)methyl)-6-chloro-, 1,1-dioxide
2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3-(((phenylmethyl)thio)methyl)-, dioxide-1,1-
2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3-[[(phenylmethyl)thio]methyl]-, 1,1-dioxide
3-((Benzylthio)methyl)-6-chloro-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
3-Benzylthiomethyl-6-chloro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
3-Benzylthiomethyl-6-chloro-7-sulfamoyl-1,2,4-benzothiadiazine 1,1-dioxide
Aquatag
Benzothiazide
Dihydrex
Diucen
Diucene
Edemex
Exna
Exosalt
Fovane
Freeuril
HyDrine
Lemazide
Naclex
P 1393
Pfizer 1393
Proaqua
Regulon
Urese

**Inchi:** InChI=1S/C15H14ClN3O4S3/c16-11-6-12-14(7-13(11)25(17,20)21)26(22,23)19-15(18-12

**InchiKey:** NDTSRXAMMQDVSW-UHFFFAOYSA-N

**Formula:** C15H14ClN3O4S3

**SMILES:** NS(=O)(=O)c1cc2c(cc1Cl)NC(CSCc1ccccc1)=NS2(=O)=O

**Mol. weight [g/mol]:** 431.94

**CAS:** 91-33-8

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -290.17 | kJ/mol | Joback Method |
| hf | -515.60 | kJ/mol | Joback Method |
| hfus | 67.85 | kJ/mol | Joback Method |

| | | | |
|---|---|---|---|
| hvap | 127.95 | kJ/mol | Joback Method |
| log10ws | -4.46 | | Aqueous Solubility Prediction Method |
| logp | 2.433 | | Crippen Method |
| mcvol | 274.240 | ml/mol | McGowan Method |
| pc | 4553.06 | kPa | Joback Method |
| rinpol | 2680.00 | | NIST Webbook |
| rinpol | 2680.00 | | NIST Webbook |
| tb | 986.32 | K | Joback Method |
| tc | 1247.77 | K | Joback Method |
| tf | 504.65 | K | Aqueous Solubility Prediction Method |
| vc | 1.058 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 780.07 | J/mol×K | 986.32 | Joback Method |
| cpg | 786.90 | J/mol×K | 1029.90 | Joback Method |
| cpg | 791.73 | J/mol×K | 1073.47 | Joback Method |
| cpg | 794.56 | J/mol×K | 1117.05 | Joback Method |
| cpg | 795.41 | J/mol×K | 1160.62 | Joback Method |
| cpg | 794.30 | J/mol×K | 1204.20 | Joback Method |
| cpg | 791.24 | J/mol×K | 1247.77 | Joback Method |

# Sources

**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/AqueousDataset003.xlsx/351830174/AqueousDa

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

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C91338&Units=SI

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |