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)N=C(CSCc1ccccc1)NS2(=O)=O

Mol. weight [g/mol]: 431.95

Physical Properties

Property code	Value	Unit	Source
hfus	67.85	kJ/mol	Joback Method
log10ws	-4.46		Aqueous Solubility Prediction Method
logp	2.243		Crippen Method
mcvol	274.240	ml/mol	McGowan Method

rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tf	504.65	K	Aqueous Solubility Prediction 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

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

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

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

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

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point