2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-, 1,1-dioxide

Other names: 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
Chlorothiazide
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]: 295.73

Physical Properties

Property code	Value	Unit	Source
hfus	49.35	kJ/mol	Joback Method
log10ws	-3.05		Aqueous Solubility Prediction Method
log10ws	-3.05		Estimated Solubility Method
logp	-0.061		Crippen Method
mcvol	168.930	ml/mol	McGowan Method
tf	530.02	K	Cheméo Relay (1.0)

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58946&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
tf:	Normal melting (fusion) point