Trichlormethiazide

Other names:

2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3-(dichloromethyl)-3,4-dihydro-, 1,1-dioxide
3-(Dichloromethyl)-6-chloro-7-sulfamoyl-3,4-dihydro-1,2,4-benzothiadiazine 1,1-dioxide
3-Dichloromethyl-6-chloro-7-sulfamyl-3,4-dihydro-1,2,4-benzothiadiazine 1,1-dioxide
3-Dichloromethylhydrochlorothiazide
6-Chloro-3-(dichloromethyl)-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
6-Chloro-3-(dichloromethyl)-3,4-dihydro-2H-1,2,4-thiadiazine-7-sulfonamide 1,1-dioxide
6-Chloro-3-(dichloromethyl)3,4-dihydro-7-sulfamoyl-1,2,4-benzothiadiazine-1,1-dioxide
6-Chloro-3-(dichloromethyl)3,4-dihydro-7-sulfamyl-1,2,4-benzothiadiazine-1,1-dioxide
Achletin
Anatran
Anistadin
Aponorin
Carvacron
Chlopolidine
Ciba 7057-Su
Cretonin
Diu-Hydrin
Diurazida
Diurese
Diuroral
Esmarin
Eurinol
Fluitran
Flurese
Flutra
Gangesol
Hydrotrichlorothiazide
Intromene
Isestran
Kubacron
Metahydrin
Metatensin
NSC 61560
Nakva
Naqua
Naquasone
Naquival
Salurin
Schebitran
Tachionin

	Tolcasone
	Trichlormetazid
	Trichlormethiazid
	Trichloromethiadiazide
	Trichloromethiazide
	Triclordiuride
	Triclormetiazide
	Triflumen
Inchi:	InChI=1S/C8H8Cl3N3O4S2/c9-3-1-4-6(2-5(3)19(12,15)16)20(17,18)14-8(13-4)7(10)11/h
InchiKey:	LMJSLTNSBFUCMU-UHFFFAOYSA-N
Formula:	C8H8Cl3N3O4S2
SMILES:	NS(=O)(=O)c1cc2c(cc1Cl)NC(C(Cl)Cl)NS2(=O)=O
Mol. weight [g/mol]:	380.66
CAS:	133-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-578.05	kJ/mol	Joback Method
hf	-786.09	kJ/mol	Joback Method
hfus	61.11	kJ/mol	Joback Method
hvap	110.94	kJ/mol	Joback Method
log10ws	-2.68		Estimated Solubility Method
logp	0.821		Crippen Method
mcvol	211.800	ml/mol	McGowan Method
pc	6359.24	kPa	Joback Method
tb	791.16	K	Joback Method
tc	1034.13	K	Joback Method
tf	752.57	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.99	J/mol×K	791.16	Joback Method
cpg	521.45	J/mol×K	831.65	Joback Method
cpg	529.72	J/mol×K	872.15	Joback Method

cpg	536.78	J/mol×K	912.64	Joback Method
cpg	542.63	J/mol×K	953.14	Joback Method
cpg	547.27	J/mol×K	993.63	Joback Method
cpg	550.69	J/mol×K	1034.13	Joback Method

Sources

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=C133675&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume