METOLAZONE

Other names: 2-Methyl-3-o-tolyl-6-sulfamyl-7-chloro-1,2,3,4-tetrahydro-4-quinazolinone
6-Quinazolinesulfonamide, 1,2,3,4-tetrahydro-7-chloro-2-methyl-4-oxo-3-o-tolyl-
6-Quinazolinesulfonamide,
7-chloro-1,2,3,4-tetrahydro-2-methyl-3-(2-methylphenyl)-4-oxo-
6-Quinazolinesulfonamide, 7-chloro-1,2,3,4-tetrahydro-2-methyl-4-oxo-3-o-tolyl-
7-Chloro-1,2,3,4-tetrahydro-2-methyl-3-(2-methylphenyl)-4-oxo-6-quinazolinesulfonamide
7-Chloro-1,2,3,4-tetrahydro-2-methyl-4-oxo-3-o-tolyl-6-quinazolinesulfonamide
7-chloro-2-methyl-3-(2-methylphenyl)-4-oxo-1,2-dihydroquinazoline-6-sulfonamide
Diulo
Metalazone
Metalozone
Metenix
Mykrox
Oldren
SR 720-22
Xuret
Zaroxolyn

Inchi: InChI=1S/C16H16ClN3O3S/c1-9-5-3-4-6-14(9)20-10(2)19-13-8-12(17)15(24(18,22)23)7-

InchiKey: AQCHWTWZEMGIFD-UHFFFAOYSA-N

Formula: C16H16ClN3O3S

SMILES: Cc1ccccc1N1C(=O)c2cc(S(N)(=O)=O)c(Cl)cc2NC1C

Mol. weight [g/mol]: 365.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Aqueous Solubility Prediction Method
log10ws	-3.78		Estimated Solubility Method
logp	2.714		Crippen Method
mcvol	249.760	ml/mol	McGowan Method
tf	527.82	K	Aqueous Solubility Prediction Method

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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=C17560519&Units=SI

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):

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point