1,2-Benzisothiazolin-3-one, 2-(0-tolylsulfonyl)-, 1,1-dioxide

Inchi: InChI=1S/C14H11NO5S2/c1-10-6-2-4-8-12(10)21(17,18)15-14(16)11-7-3-5-9-13(11)22(1

InchiKey: MVYMEXWAIRLDNP-UHFFFAOYSA-N

Formula: C14H11NO5S2

SMILES: Cc1ccccc1S(=O)(=O)N1C(=O)c2ccccc2S1(=O)=O

Mol. weight [g/mol]: 337.37

CAS: 116400-87-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	1.528		Crippen Method
mcvol	217.470	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116400874&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume