1,2-Benzisothiazol-3(2H)-one, 2-methyl-, 1,1-dioxide

Other names: 1,2-Benzisothiazolin-3-one, 2-methyl-, 1,1-dioxide
N-Methylsaccharin
2-Methyl-1,2-benzisothiazole-3(2H)-one-1,1-dioxide
2-Methyl-1,2-benzisothiazol-3(2H)-one 1,1-dioxide
Saccharin methylated
NSC 39120
Saccharin methylated (major component)

Inchi: InChI=1S/C8H7NO3S/c1-9-8(10)6-4-2-3-5-7(6)13(9,11)12/h2-5H,1H3

InchiKey: DDIIAJRLFATEEE-UHFFFAOYSA-N

Formula: C8H7NO3S

SMILES: CN1C(=O)c2ccccc2S1(=O)=O

Mol. weight [g/mol]: 197.21

CAS: 15448-99-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.36		Crippen Method
logp	0.461		Crippen Method
mcvol	128.600	ml/mol	McGowan Method
rinpol	1655.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1674.00		NIST Webbook

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=C15448994&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
rinpol:	Non-polar retention indices