

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/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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