

3-Methyl-3H-benzothiazol-2-one

Other names:	2-Benzothiazolinone, N-methyl-
Inchi:	InChI=1S/C8H7NOS/c1-9-6-4-2-3-5-7(6)11-8(9)10/h2-5H,1H3
InchiKey:	LSMMRJUHLKJNLR-UHFFFAOYSA-N
Formula:	C8H7NOS
SMILES:	Cn1c(=O)sc2ccccc21
Mol. weight [g/mol]:	165.21
CAS:	2786-62-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	1.600		Crippen Method
mcvol	116.860	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=C2786621&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

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