

3(2H)-Isothiazolone, 2-methyl-

Other names:	2-Methyl-3(2H)-isothiazolone 2-methyl-2H-isothiazol-3-one
Inchi:	InChI=1S/C4H5NOS/c1-5-4(6)2-3-7-5/h2-3H,1H3
InchiKey:	BEGLCMHJXHIJLR-UHFFFAOYSA-N
Formula:	C4H5NOS
SMILES:	Cn1sccc1=O
Mol. weight [g/mol]:	115.15
CAS:	2682-20-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	0.447		Crippen Method
mcvol	79.960	ml/mol	McGowan Method
rinpol	1431.00		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=C2682204&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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