

4-Methylthiomorpholine-1,1-dioxide

Other names:	N-Methyltetrahydro-1,4-thiazine-S-oxide Thiomorpholine, 4-methyl-, 1,1-dioxide
Inchi:	InChI=1S/C5H11NO2S/c1-6-2-4-9(7,8)5-3-6/h2-5H2,1H3
InchiKey:	ULZCOWMSBOJCLT-UHFFFAOYSA-N
Formula:	C5H11NO2S
SMILES:	CN1CCS(=O)(=O)CC1
Mol. weight [g/mol]:	149.21
CAS:	25343-91-3

Physical Properties

Property code	Value	Unit	Source
log10ws	0.79		Crippen Method
logp	-0.653		Crippen Method
mcvol	108.520	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25343913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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