

N-Methylthiomorpholine

Inchi: InChI=1S/C5H11NS/c1-6-2-4-7-5-3-6/h2-5H2,1H3
InchiKey: KDTVWEHAAISPW-UHFFFAOYSA-N
Formula: C5H11NS
SMILES: CN1CCSCC1
Mol. weight [g/mol]: 117.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.26		Crippen Method
logp	0.665		Crippen Method
mcvol	96.780	ml/mol	McGowan Method
rinpola	969.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R346040&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinpola: Non-polar retention indices

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