

3-Pyridinol, 6-methyl-2-(methylthio)-

Inchi:	InChI=1S/C7H9NOS/c1-5-3-4-6(9)7(8-5)10-2/h3-4,9H,1-2H3
InchiKey:	IWWGZBKCVIXGMG-UHFFFAOYSA-N
Formula:	C7H9NOS
SMILES:	CSc1nc(C)ccc1O
Mol. weight [g/mol]:	155.22
CAS:	23003-25-0

Physical Properties

Property code	Value	Unit	Source
ie	8.24 ± 0.05	eV	NIST Webbook
log10ws	-2.00		Crippen Method
logp	1.818		Crippen Method
mcvol	117.930	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23003250&Units=SI

Legend

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

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<https://www.chemeo.com/cid/68-865-7/3-Pyridinol-6-methyl-2-methylthio.pdf>

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