2(1H)-Pyridinethione, 1-methyl-

Other names:	N-Methyl-2-pyridinethione
	1-Methyl-2-pyridinethione
	1-Methyl-2-thiopyridone
	1-Methyl-2(1H)-pyridinethione
	N-Methylthiopyridone-2
Inchi:	InChI=1S/C6H7NS/c1-7-5-3-2-4-6(7)8/h2-5H,1H3
InchiKey:	UHOAUPKGWPQNDM-UHFFFAOYSA-N
Formula:	C6H7NS
SMILES:	Cn1ccccc1=S
Mol. weight [g/mol]:	125.19
CAS:	2044-27-1

Physical Properties

Property code	Value	Unit	Source
ie	7.84 ± 0.02	eV	NIST Webbook
ie	7.69 ± 0.03	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	1.755		Crippen Method
mcvol	97.970	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=C2044271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume