

2(1H)-Pyridinethione

Other names:	Pyrid-2-thione
	2-Mercaptopyridine
	2-Pyridinethiol
	2-Pyridinethione
	2-Thiopyridine
	2-Thiopyridone
	2-Pyridyl mercaptan
	pyridine-2-thiol
Inchi:	InChI=1S/C5H5NS/c7-5-3-1-2-4-6-5/h1-4H,(H,6,7)
InchiKey:	WHMDPDGBKYUEMW-UHFFFAOYSA-N
Formula:	C5H5NS
SMILES:	S=c1cccc[nH]1
Mol. weight [g/mol]:	111.17
CAS:	2637-34-5

Physical Properties

Property code	Value	Unit	Source
ie	7.77	eV	NIST Webbook
ie	7.80 ± 0.03	eV	NIST Webbook
log10ws	-1.54		Crippen Method
logp	1.262		Crippen Method
mcvol	83.880	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C2637345&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/17-565-6/2-1H-Pyridinethione.pdf>

Generated by Cheméo on 2024-04-23 13:38:01.850265777 +0000 UTC m=+16168730.770843090.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.