2(1H)-Pyridinethione, 3-hydroxy-6-methyl-

Inchi: InChI=1S/C6H7NOS/c1-4-2-3-5(8)6(9)7-4/h2-3,8H,1H3,(H,7,9)
InchiKey: KWMLIEDLOLUHHQ-UHFFFAOYSA-N
Formula: C6H7NOS
SMILES: Cc1ccc(O)c(S)n1
Mol. weight [g/mol]: 141.19
CAS: 22989-67-9

Physical Properties

Property code	Value	Unit	Source
ie	8.04 ± 0.05	eV	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.384		Crippen Method
mcvol	103.840	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C22989679&Units=SI

Legend

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

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