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

Inchi: InChI=1S/C8H11NOS/c1-3-9-6(2)4-5-7(10)8(9)11/h4-5,10H,3H2,1-2H3
InchiKey: BJEVGGTVTRCGSV-UHFFFAOYSA-N
Formula: C8H11NOS
SMILES: CCn1c(C)ccc(O)c1=S
Mol. weight [g/mol]: 169.24
CAS: 24207-15-6

Physical Properties

Property code	Value	Unit	Source
ie	7.75 ± 0.05	eV	NIST Webbook
log10ws	-2.61		Crippen Method
logp	2.252		Crippen Method
mcvol	132.020	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24207156&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.