3-Pyridinol, 2-(methylthio)-, acetate (ester)

Inchi: InChI=1S/C8H9NO2S/c1-6(10)11-7-4-3-5-9-8(7)12-2/h3-5H,1-2H3
InchiKey: ROICIIOLSQXXLP-UHFFFAOYSA-N
Formula: C8H9NO2S
SMILES: CSc1ncccc1OC(C)=O
Mol. weight [g/mol]: 183.23
CAS: 42715-30-0

Physical Properties

Property code	Value	Unit	Source
ie	7.91 ± 0.05	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	1.729		Crippen Method
mcvol	133.590	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=C42715300&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

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