

# Ethyl-2-(3-methylpyrazinyl mercapto) acetate

**Inchi:** InChI=1S/C9H12N2O2S/c1-3-13-8(12)6-14-9-7(2)10-4-5-11-9/h4-5H,3,6H2,1-2H3  
**InchiKey:** WXCGBBGPBKSPNQ-UHFFFAOYSA-N  
**Formula:** C9H12N2O2S  
**SMILES:** CCOC(=O)CSc1nccnc1C  
**Mol. weight [g/mol]:** 212.27

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	1.440		Crippen Method
mcvol	157.660	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=B6002793&Units=SI>

## Legend

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

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