

# 2-(T-dodecyl mercapto)-3-methyl pyrazine

**Inchi:** InChI=1S/C17H30N2S/c1-5-6-7-8-9-10-11-12-17(3,4)20-16-15(2)18-13-14-19-16/h13-14  
**InchiKey:** UASZAUZXOQSTHZ-UHFFFAOYSA-N  
**Formula:** C17H30N2S  
**SMILES:** CCCCCCCCC(C)(C)Sc1nccnc1C  
**Mol. weight [g/mol]:** 294.50  
**CAS:** 116323-36-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.94		Crippen Method
logp	5.796		Crippen Method
mcvol	262.940	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C116323365&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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