

# Pyrazine, 3-methylthio-2-pentyl

**Other names:** Pyrazine, 2-(methylthio)-3-pentyl  
**Inchi:** InChI=1S/C10H16N2S/c1-3-4-5-6-9-10(13-2)12-8-7-11-9/h7-8H,3-6H2,1-2H3  
**InchiKey:** QPQMKGUVJKDKOV-UHFFFAOYSA-N  
**Formula:** C10H16N2S  
**SMILES:** CCCCCc1nccnc1SC  
**Mol. weight [g/mol]:** 196.31

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.931		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1970.00		NIST Webbook

## Sources

**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=R43770&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices  
**ripol:** Polar retention indices

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