

# Pyrazine, 2-decyl-3-methylthio

**Inchi:** InChI=1S/C15H26N2S/c1-3-4-5-6-7-8-9-10-11-14-15(18-2)17-13-12-16-14/h12-13H,3-11  
**InchiKey:** KPAZGTKAMSIERT-UHFFFAOYSA-N  
**Formula:** C15H26N2S  
**SMILES:** CCCCCCCCCc1nccnc1SC  
**Mol. weight [g/mol]:** 266.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	4.882		Crippen Method
mcvol	234.760	ml/mol	McGowan Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
ripol	2499.00		NIST Webbook
ripol	2499.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R43421&Units=SI>  
**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)

## 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

Latest version available from:

<https://www.cheméo.com/cid/91-219-8/Pyrazine-2-decyl-3-methylthio.pdf>

Generated by Cheméo on 2024-04-29 10:19:20.118247188 +0000 UTC m=+16675209.038824503.

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