

# Pyrazine, 2-octyl-3-phenylthio

**Inchi:** InChI=1S/C18H24N2S/c1-2-3-4-5-6-10-13-17-18(20-15-14-19-17)21-16-11-8-7-9-12-16/H  
**InchiKey:** KGQCBIZAFKZZQC-UHFFFAOYSA-N  
**Formula:** C18H24N2S  
**SMILES:** CCCCCCCCc1nccnc1Sc1cccc1  
**Mol. weight [g/mol]:** 300.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.73		Crippen Method
logp	5.531		Crippen Method
mcvol	253.270	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
ripol	3016.00		NIST Webbook
ripol	3016.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R43574&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

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