

# Pyrazine, 2-ethyl-3-ethylthio

**Inchi:** InChI=1S/C8H12N2S/c1-3-7-8(11-4-2)10-6-5-9-7/h5-6H,3-4H2,1-2H3  
**InchiKey:** FDIFCVWENOSOQZ-UHFFFAOYSA-N  
**Formula:** C8H12N2S  
**SMILES:** CCSc1nccnc1CC  
**Mol. weight [g/mol]:** 168.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	2.151		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook
ripol	1723.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R43435&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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