

# Pyrazine, (methylthio)-

<b>Other names:</b>	2-(Methylsulfanyl)pyrazine (Methylthio)pyrazine Methyl pyrazinyl sulfide
<b>Inchi:</b>	InChI=1S/C5H6N2S/c1-8-5-4-6-2-3-7-5/h2-4H,1H3
<b>InchiKey:</b>	KBPBOWBQRUXMFV-UHFFFAOYSA-N
<b>Formula:</b>	C5H6N2S
<b>SMILES:</b>	CS <sub>c</sub> 1cncn1
<b>Mol. weight [g/mol]:</b>	126.18
<b>CAS:</b>	21948-70-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.198		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
ripol	1600.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21948709&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21948709&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

**rinpol:** Non-polar retention indices

**ripol:** Polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/39-326-7/Pyrazine-methylthio.pdf>

Generated by Cheméo on 2024-05-02 15:04:11.659132582 +0000 UTC m=+16951500.579709908.

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