

# 2-(Methylthio)methyl-3,5,6-trimethylpyrazine

<b>Inchi:</b>	InChI=1S/C9H14N2S/c1-6-7(2)11-9(5-12-4)8(3)10-6/h5H2,1-4H3
<b>InchiKey:</b>	FUDCPZZFJNUELV-UHFFFAOYSA-N
<b>Formula:</b>	C9H14N2S
<b>SMILES:</b>	CSCc1nc(C)c(C)nc1C
<b>Mol. weight [g/mol]:</b>	182.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	2.265		Crippen Method
mcvol	150.220	ml/mol	McGowan Method
ripol	2060.00		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=R319701&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R319701&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
<b>ripol:</b>	Polar retention indices

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