

# 2-Benzylmercapto-3-methyl pyrazine

<b>Inchi:</b>	InChI=1S/C12H12N2S/c1-10-12(14-8-7-13-10)15-9-11-5-3-2-4-6-11/h2-8H,9H2,1H3
<b>InchiKey:</b>	YFTXLZYURWUCQR-UHFFFAOYSA-N
<b>Formula:</b>	C12H12N2S
<b>SMILES:</b>	Cc1nccnc1SCc1ccccc1
<b>Mol. weight [g/mol]:</b>	216.30
<b>CAS:</b>	74990-49-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	3.077		Crippen Method
mcvol	168.730	ml/mol	McGowan Method

## Sources

<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=C74990491&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C74990491&amp;Units=SI</a>
<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>

## 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

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