

# 2-Furylmethylsulfide

<b>Other names:</b>	Methyl furfuryl sulfide 2-Methylsulfanyl-furan Furan,2-(methylthio)-
<b>Inchi:</b>	InChI=1S/C5H6OS/c1-7-5-3-2-4-6-5/h2-4H,1H3
<b>InchiKey:</b>	QNQUVXCNWQTHHY-UHFFFAOYSA-N
<b>Formula:</b>	C5H6OS
<b>SMILES:</b>	CSc1ccco1
<b>Mol. weight [g/mol]:</b>	114.17
<b>CAS:</b>	13129-38-9

## Physical Properties

Property code	Value	Unit	Source
ie	8.58 ± 0.05	eV	NIST Webbook
log10ws	-5.95		Crippen Method
logp	2.002		Crippen Method
mcpol	84.070	ml/mol	McGowan Method
ripol	902.00		NIST Webbook
ripol	894.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	865.00		NIST Webbook
ripol	865.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1492.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13129389&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13129389&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>ie:</b>	Ionization energy
<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>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices

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