

# 1H-Indole, 4-methoxy-

<b>Other names:</b>	Indole, 4-methoxy- 4-Methoxyindole 4-Methoxy-1H-indole
<b>Inchi:</b>	InChI=1S/C9H9NO/c1-11-9-4-2-3-8-7(9)5-6-10-8/h2-6,10H,1H3
<b>InchiKey:</b>	LUNOXNMCFPFPMO-UHFFFAOYSA-N
<b>Formula:</b>	C9H9NO
<b>SMILES:</b>	<chem>COc1cccc2[nH]ccc12</chem>
<b>Mol. weight [g/mol]:</b>	147.17
<b>CAS:</b>	4837-90-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.695		Crippen Method
mcvol	114.600	ml/mol	McGowan Method
ripol	2114.00		NIST Webbook
ripol	2114.00		NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.20	K	3.20	NIST Webbook

## 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=C4837905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4837905&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
<b>ripol:</b>	Polar retention indices
<b>tbrp:</b>	Boiling point at reduced pressure

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