

1H-Indole, 5-methoxy-

Other names:	Femedol Indole, 5-methoxy- 5-Methoxyindole 5-Methoxy-1H-indole Methoxy-5 indole indol-5-yl methyl ether
Inchi:	InChI=1S/C9H9NO/c1-11-8-2-3-9-7(6-8)4-5-10-9/h2-6,10H,1H3
InchiKey:	DWAQDRSOVMLGRQ-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	<chem>COc1ccc2[nH]ccc2c1</chem>
Mol. weight [g/mol]:	147.17
CAS:	1006-94-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.695		Crippen Method
mccvol	114.600	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.20	K	2.30	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1006946&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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