

# 1H-Indole, 6-methyl-

<b>Other names:</b>	6-Methylindole Indole, 6-methyl-
<b>Inchi:</b>	InChI=1S/C9H9N/c1-7-2-3-8-4-5-10-9(8)6-7/h2-6,10H,1H3
<b>InchiKey:</b>	ONYNOPPOVKYGRS-UHFFFAOYSA-N
<b>Formula:</b>	C9H9N
<b>SMILES:</b>	Cc1ccc2cc[nH]c2c1
<b>Mol. weight [g/mol]:</b>	131.17
<b>CAS:</b>	3420-02-8

## Physical Properties

Property code	Value	Unit	Source
ie	7.54 ± 0.01	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	1.994		Crippen Method
mcvol	108.730	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	0.70	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39985e+01
Coeff. B	-4.20390e+03
Coeff. C	-8.74780e+01
Temperature range (K), min.	394.09
Temperature range (K), max.	571.40

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## 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=C3420028&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3420028&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>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>pvap:</b>	Vapor pressure
<b>tbrp:</b>	Boiling point at reduced pressure

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