

# 1H-Indole, 2,3,5-trimethyl-

<b>Other names:</b>	Indole, 2,3,5-trimethyl- 2,3,5-Trimethylindole
<b>Inchi:</b>	InChI=1S/C11H13N/c1-7-4-5-11-10(6-7)8(2)9(3)12-11/h4-6,12H,1-3H3
<b>InchiKey:</b>	HOFNMMIHFZBKPW-UHFFFAOYSA-N
<b>Formula:</b>	C11H13N
<b>SMILES:</b>	<chem>Cc1ccc2[nH]c(C)c(C)c2c1</chem>
<b>Mol. weight [g/mol]:</b>	159.23
<b>CAS:</b>	21296-92-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	2.611		Crippen Method
mcvol	136.910	ml/mol	McGowan Method
rinpol	273.61		NIST Webbook
rinpol	272.57		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21296924&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21296924&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/28-201-7/1H-Indole-2-3-5-trimethyl.pdf>

Generated by Cheméo on 2024-04-20 14:29:39.0391066 +0000 UTC m=+15912627.959683916.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.