

# 1H-Pyrazole, 3,5-dimethyl-1-phenyl-

<b>Other names:</b>	3,5-Dimethyl-1-phenylpyrazole 3,5-dimethyl-1-phenyl-1H-pyrazole
<b>Inchi:</b>	InChI=1S/C11H12N2/c1-9-8-10(2)13(12-9)11-6-4-3-5-7-11/h3-8H,1-2H3
<b>InchiKey:</b>	ULPMPUPEFBDQQA-UHFFFAOYSA-N
<b>Formula:</b>	C11H12N2
<b>SMILES:</b>	<chem>Cc1cc(C)n(-c2ccccc2)n1</chem>
<b>Mol. weight [g/mol]:</b>	172.23
<b>CAS:</b>	1131-16-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.489		Crippen Method
mcpvol	142.590	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.70	K	1.70	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=C1131164&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1131164&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>tbrp:</b>	Boiling point at reduced pressure

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