

# 1H-Pyrrole, 1-(phenylmethyl)-

<b>Other names:</b>	Pyrrole, 1-benzyl- N-Benzylpyrrole 1-Benzylpyrrole
<b>Inchi:</b>	InChI=1S/C11H11N/c1-2-6-11(7-3-1)10-12-8-4-5-9-12/h1-9H,10H2
<b>InchiKey:</b>	FNEQHKCQXDKYEO-UHFFFAOYSA-N
<b>Formula:</b>	C11H11N
<b>SMILES:</b>	<chem>c1ccc(Cn2cccc2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	157.21
<b>CAS:</b>	2051-97-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	2.536		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
tf	288.00 ± 2.00	K	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.20	K	3.60	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=C2051970&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051970&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>tbrp:</b>	Boiling point at reduced pressure
<b>tf:</b>	Normal melting (fusion) point

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