

# Pyrimidine, 5-(4-methylphenyl)-

<b>Inchi:</b>	InChI=1S/C11H10N2/c1-9-2-4-10(5-3-9)11-6-12-8-13-7-11/h2-8H,1H3
<b>InchiKey:</b>	HMIDRMDGUSXDTP-UHFFFAOYSA-N
<b>Formula:</b>	C11H10N2
<b>SMILES:</b>	Cc1ccc(-c2cncnc2)cc1
<b>Mol. weight [g/mol]:</b>	170.21

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	2.452		Crippen Method
mcvol	138.290	ml/mol	McGowan Method
rinpola	1649.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380550&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380550&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>rinpola:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/78-927-7/Pyrimidine-5-4-methylphenyl.pdf>

Generated by Cheméo on 2024-04-28 06:08:09.730070484 +0000 UTC m=+16573738.650647796.

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