

Pyridine, 2-methyl-5-phenyl-

Other names:	2-Picoline, 5-phenyl- 2-Methyl-5-phenylpyridine
Inchi:	InChI=1S/C12H11N/c1-10-7-8-12(9-13-10)11-5-3-2-4-6-11/h2-9H,1H3
InchiKey:	JXNAIOCJWBJGFQ-UHFFFAOYSA-N
Formula:	C12H11N
SMILES:	<chem>Cc1ccc(-c2cccc2)cn1</chem>
Mol. weight [g/mol]:	169.22
CAS:	3256-88-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	3.057		Crippen Method
mcvol	142.400	ml/mol	McGowan Method
rinpol	1513.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2274.00		NIST Webbook
ripol	2332.00		NIST Webbook
ripol	2282.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3256880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

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