

Pyridine, 3-phenyl-4-propyl-

Other names:	3-phenyl-4-propylpyridine
Inchi:	InChI=1S/C14H15N/c1-2-6-12-9-10-15-11-14(12)13-7-4-3-5-8-13/h3-5,7-11H,2,6H2,1H3
InchiKey:	MDEOSZGDWLTQLL-UHFFFAOYSA-N
Formula:	C14H15N
SMILES:	CCCc1ccncc1-c1ccccc1
Mol. weight [g/mol]:	197.28
CAS:	53911-35-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	3.701		Crippen Method
mcvol	170.580	ml/mol	McGowan Method
rinpol	1615.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53911356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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