

1-(3-Phenyl-2-propenyl)pyridinium

Inchi:	InChI=1S/C14H14N/c1-3-8-14(9-4-1)10-7-13-15-11-5-2-6-12-15/h1-12H,13H2/q+1/b10-7
InchiKey:	BLGKHANBLJGCII-JXMROGBWSA-N
Formula:	C14H14N
SMILES:	<chem>C(=Cc1ccccc1)C[n+]1ccccc1</chem>
Mol. weight [g/mol]:	196.27
CAS:	125713-88-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	2.688		Crippen Method
mcvol	168.430	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C125713884&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

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<https://www.chemeo.com/cid/41-062-7/1-3-Phenyl-2-propenyl-pyridinium.pdf>

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