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: C(=Cc1ccccc1)C[n+]1ccccc1
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/ci990307l
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