

2-(1-Phenylethenyl)pyridine

Other names:	Pyridine,2-(1-phenylethenyl)- 1-Phenyl-1-(2-pyridyl)ethylene
Inchi:	InChI=1S/C13H11N/c1-11(12-7-3-2-4-8-12)13-9-5-6-10-14-13/h2-10H,1H2
InchiKey:	WLFQFTSISRWCNV-UHFFFAOYSA-N
Formula:	C13H11N
SMILES:	C=C(c1ccccc1)c1cccn1
Mol. weight [g/mol]:	181.23
CAS:	15260-65-8

Physical Properties

Property code	Value	Unit	Source
ie	8.65	eV	NIST Webbook
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log10ws	-3.78		Crippen Method
logp	3.143		Crippen Method
mcvol	152.190	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15260658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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