4-(2-Phenylvinyl)pyridine, trans-

Other names:	4-(2-Phenylethenyl)pyridine, (E)
	Pyridine, 4-(2-phenylethenyl)-, (E)-
	Pyridine, trans-4-(2-phenylethenyl)-
Inchi:	InChI=1S/C13H11N/c1-2-4-12(5-3-1)6-7-13-8-10-14-11-9-13/h1-11H/b7-6+
InchiKey:	QKHRGPYNTXRMSL-VOTSOKGWSA-N
Formula:	C13H11N
SMILES:	C(=Cc1ccncc1)c1ccccc1
Mol. weight [g/mol]:	181.23
CAS:	5097-93-8

Physical Properties

Property code	Value	Unit	Source
ie	8.36	eV	NIST Webbook
ie	8.34 ± 0.05	eV	NIST Webbook
log10ws	-3.84		Crippen Method
logp	3.252		Crippen Method
mcvol	152.190	ml/mol	McGowan Method

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=C5097938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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