

Pyridine, 2-(2-(2-nitrophenyl)ethenyl)-, trans

Other names:	(E)-2-(2-Nitrophenylethenyl)pyridine
Inchi:	InChI=1S/C13H10N2O2/c16-15(17)13-7-2-1-5-11(13)8-9-12-6-3-4-10-14-12/h1-10H/b9-8
InchiKey:	YADNATDOWRSAOC-CMDGGOBGSA-N
Formula:	C13H10N2O2
SMILES:	O=[N+](O-)c1cccc1C=Cc1ccccn1
Mol. weight [g/mol]:	226.23
CAS:	77340-84-2

Physical Properties

Property code	Value	Unit	Source
ie	8.30	eV	NIST Webbook
log10ws	-4.49		Crippen Method
logp	3.160		Crippen Method
mcvol	169.610	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=C77340842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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<https://www.chemeo.com/cid/11-567-0/Pyridine-2-2-2-nitrophenyl-ethenyl-trans.pdf>

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