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-])c1ccccc1C=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/ci990307l

Legend

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