

trans-2,4'-vinylenedipyridine

Other names: Pyridine, 4-(2-(pyridyl-4)ethenyl)-, trans-
Inchi: InChI=1S/C12H10N2/c1-2-8-14-12(3-1)5-4-11-6-9-13-10-7-11/h1-10H/b5-4+
InchiKey: RETWYDZOYDJBIX-SNAWJCMRSA-N
Formula: C12H10N2
SMILES: C(=Cc1ccccn1)c1ccncc1
Mol. weight [g/mol]: 182.22
CAS: 14802-41-6

Physical Properties

Property code	Value	Unit	Source
ie	8.50 ± 0.03	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	2.647		Crippen Method
mcvol	148.080	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=C14802416&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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