

5,5'-Bipyrimidine

Inchi: InChI=1S/C8H6N4/c1-7(2-10-5-9-1)8-3-11-6-12-4-8/h1-6H
InchiKey: NYRJZUWFXMJYAP-UHFFFAOYSA-N
Formula: C8H6N4
SMILES: c1ncc(-c2cncnc2)cn1
Mol. weight [g/mol]: 158.16
CAS: 56598-46-0

Physical Properties

Property code	Value	Unit	Source
ie	9.00	eV	NIST Webbook
ie	9.68	eV	NIST Webbook
log10ws	-3.14		Crippen Method
logp	0.934		Crippen Method
mcvol	115.980	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56598460&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/57-723-6/5-5-Bipyrimidine.pdf>

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