Isophosphinoline, 3-methyl-

Inchi: InChI=1S/C10H9P/c1-8-6-9-4-2-3-5-10(9)7-11-8/h2-7H,1H3
InchiKey: MLFHRAFKAKVRKS-UHFFFAOYSA-N
Formula: C10H9P
SMILES: Cc1cc2ccccc2cp1
Mol. weight [g/mol]: 160.15
CAS: 49622-63-1

Physical Properties

Property code	Value	Unit	Source
ie	7.96	eV	NIST Webbook
log10ws	-0.75		Crippen Method
logp	3.728		Crippen Method
mcvol	129.000	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=C49622631&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.