

Isophosphinoline

Inchi: InChI=1S/C9H7P/c1-2-4-9-7-10-6-5-8(9)3-1/h1-7H
InchiKey: ODZILJDRJCJHKM-UHFFFAOYSA-N
Formula: C9H7P
SMILES: c1ccc2cpccc2c1
Mol. weight [g/mol]: 146.13
CAS: 253-37-2

Physical Properties

Property code	Value	Unit	Source
ie	8.04	eV	NIST Webbook
log10ws	-0.27		Crippen Method
logp	3.420		Crippen Method
mcvol	114.910	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C253372&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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/48-658-9/Isophosphinoline.pdf>

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