Isophosphinoline, 1,3-dimethyl-

Inchi: InChI=1S/C11H11P/c1-8-7-10-5-3-4-6-11(10)9(2)12-8/h3-7H,1-2H3
InchiKey: SEWWWRZAMOFLHW-UHFFFAOYSA-N
Formula: C11H11P
SMILES: Cc1cc2ccccc2c(C)p1
Mol. weight [g/mol]: 174.18
CAS: 57328-61-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Crippen Method
logp	4.037		Crippen Method
mcvol	143.090	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57328617&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

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