Phosphinic acid, phenyl-, isobutyl ester

Inchi: InChI=1S/C10H15O2P/c1-9(2)8-12-13(11)10-6-4-3-5-7-10/h3-7,9,13H,8H2,1-2H3
InchiKey: OOCQBUVKSMIFOY-UHFFFAOYSA-N
Formula: C10H15O2P
SMILES: CC(C)CO[PH](=O)c1ccccc1
Mol. weight [g/mol]: 198.20
CAS: 13336-52-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.82		Crippen Method
logp	2.459		Crippen Method
mcvol	160.200	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13336522&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