

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/17-898-7/Phosphinic-acid-phenyl-isobutyl-ester.pdf>

Generated by Cheméo on 2024-04-23 21:02:36.018463079 +0000 UTC m=+16195404.939040395.

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