

# Phenylphosphonic acid, 2-methylpentyl octyl ester

Inchi:	InChI=1S/C20H35O3P/c1-4-6-7-8-9-13-17-22-24(21,20-15-11-10-12-16-20)23-18-19(3)1
InchiKey:	JTPRRRFZRMGMSL-UHFFFAOYSA-N
Formula:	C20H35O3P
SMILES:	CCCCCCCCOP(=O)(OCC(C)CCC)c1ccccc1
Mol. weight [g/mol]:	354.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-11.89		Crippen Method
logp	6.335		Crippen Method
mcvol	306.970	ml/mol	McGowan Method
rinpol	2393.00		NIST Webbook
rinpol	2393.00		NIST Webbook

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393262&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393262&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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