

# Phenylphosphonic acid, 2,4,4-trimethylpentyl butyl ester

Inchi:	InChI=1S/C18H31O3P/c1-6-7-13-20-22(19,17-11-9-8-10-12-17)21-15-16(2)14-18(3,4)5/h
InchiKey:	SCBNWSPIIYJGC-UHFFFAOYSA-N
Formula:	C18H31O3P
SMILES:	CCCCOP(=O)(OCC(C)CC(C)(C)C)c1ccccc1
Mol. weight [g/mol]:	326.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.81		Crippen Method
logp	5.411		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
rinpola	2098.00		NIST Webbook
rinpola	2098.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
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=U393220&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393220&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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