

# Phenylphosphonic acid, dodecyl isobutyl ester

Inchi:	InChI=1S/C22H39O3P/c1-4-5-6-7-8-9-10-11-12-16-19-24-26(23,25-20-21(2)3)22-17-14-
InchiKey:	XQHSUSAHBOHMSQ-UHFFFAOYSA-N
Formula:	C22H39O3P
SMILES:	CCCCCCCCCCCCOP(=O)(OCC(C)C)c1ccccc1
Mol. weight [g/mol]:	382.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-12.73		Crippen Method
logp	7.115		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
rinpol	2642.00		NIST Webbook
rinpol	2642.00		NIST Webbook

## Sources

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.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=U393241&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393241&amp;Units=SI</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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