

Phenylphosphonic acid, dodecyl pentyl ester

Inchi:	InChI=1S/C23H41O3P/c1-3-5-7-8-9-10-11-12-13-18-22-26-27(24,25-21-17-6-4-2)23-19-
InchiKey:	GLEXFLFYCOFQGN-UHFFFAOYSA-N
Formula:	C23H41O3P
SMILES:	CCCCCCCCCCCCOP(=O)(OCCCCC)c1ccccc1
Mol. weight [g/mol]:	396.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.39		Crippen Method
logp	7.649		Crippen Method
mcvol	349.240	ml/mol	McGowan Method
rinpol	2778.00		NIST Webbook
rinpol	2778.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393243&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
rinpol:	Non-polar retention indices

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