

Phenylphosphonic acid, 2,4,4-trimethylpentyl tridecyl ester

Inchi:	InChI=1S/C27H49O3P/c1-6-7-8-9-10-11-12-13-14-15-19-22-29-31(28,26-20-17-16-18-21)
InchiKey:	NJKMHSTZGCLTIH-UHFFFAOYSA-N
Formula:	C27H49O3P
SMILES:	CCCCCCCCCCCCOP(=O)(OCC(C)CC(C)(C)C)c1ccccc1
Mol. weight [g/mol]:	452.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.58		Crippen Method
logp	8.921		Crippen Method
mcvol	405.600	ml/mol	McGowan Method
rinsol	2986.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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