

Phosphoric acid, (1-methylethyl)phenyl diphenyl ester

Other names:	Isopropylphenyl diphenyl phosphate Propylated triphenyl phosphate Syn-O-Ad 8480
Inchi:	InChI=1S/C21H21O4P/c1-17(2)20-15-9-10-16-21(20)25-26(22,23-18-11-5-3-6-12-18)24-
InchiKey:	JJXNVYMIYBNZQX-UHFFFAOYSA-N
Formula:	C21H21O4P
SMILES:	CC(C)c1ccccc1OP(=O)(Oc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	368.36
CAS:	28108-99-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.32		Crippen Method
logp	6.455		Crippen Method
mcvol	279.410	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28108998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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