

Diphenyl o-xenyl phosphate

Other names:	Phosphoric acid, 2-biphenyl, diphenyl ester
Inchi:	InChI=1S/C24H19O4P/c25-29(26-21-14-6-2-7-15-21,27-22-16-8-3-9-17-22)28-24-19-11-
InchiKey:	QARIOUOTENZTDH-UHFFFAOYSA-N
Formula:	C24H19O4P
SMILES:	O=P(Oc1cccc1)(Oc1cccc1)Oc1cccc1-c1cccc1
Mol. weight [g/mol]:	402.38
CAS:	132-29-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.74		Crippen Method
logp	6.998		Crippen Method
mcvol	297.920	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C132296&Units=SI

Legend

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

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