Phosphorous acid, tris(4-methylphenyl) ester

Other names:	Phosphorous acid, tri-p-tolyl ester
	Tri-p-cresyl phosphite
	Tri-p-tolyl phosphite
	Tris(p-methylphenyl) phosphite
	Tris(p-tolyl) phosphite
	p-Tolyl phosphite ((C7H7O)3P)
	Phosphorous acid, tri-p-cresyl ester
	Tris(4-methylphenyl) phosphite
	NSC 4054
Inchi:	InChI=1S/C21H21O3P/c1-16-4-10-19(11-5-16)22-25(23-20-12-6-17(2)7-13-20)24-21-14-
InchiKey:	FEVFLQDDNUQKRY-UHFFFAOYSA-N
Formula:	C21H21O3P
SMILES:	Cc1ccc(OP(Oc2ccc(C)cc2)Oc2ccc(C)cc2)cc1
Mol. weight [g/mol]:	352.36
CAS:	620-42-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	6.376		Crippen Method
mcvol	273.540	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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