(Triphenylphosphoranylidene)acetaldehyde

Other names:	Formylmethylenetriphenylphosphorane
	Acetaldehyde, (triphenylphosphoranylidene)-
Inchi:	InChI=1S/C20H17OP/c21-16-17-22(18-10-4-1-5-11-18,19-12-6-2-7-13-19)20-14-8-3-9-15
InchiKey:	CQCAYWAIRTVXIY-UHFFFAOYSA-N
Formula:	C20H17OP
SMILES:	O=CC=P(c1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	304.32
CAS:	2136-75-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.39		Crippen Method
logp	2.982		Crippen Method
mcvol	243.410	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2136756&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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