

1,3-Bis(diphenylphosphino)propane

Other names:	Bis(1,3-diphenylphosphino)propane Phosphine, 1,3-propanediylbis[diphenyl- Phosphine, trimethylenebis(diphenyl- Trimethylenebis(diphenylphosphine) 1,3-Propanediylbis(diphenylphosphine) propane-1,3-diylbis(diphenylphosphine)
Inchi:	InChI=1S/C27H26P2/c1-5-14-24(15-6-1)28(25-16-7-2-8-17-25)22-13-23-29(26-18-9-3-10)
InchiKey:	LVEYOSJUKRVCCF-UHFFFAOYSA-N
Formula:	C27H26P2
SMILES:	c1ccc(P(CCCP(c2ccccc2)c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]:	412.44
CAS:	6737-42-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.79		Crippen Method
logp	5.642		Crippen Method
mcvol	337.170	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6737424&Units=SI
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

Legend

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

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