

Phosphine, 1,2-ethynediylbis[diphenyl-

Other names:	Phosphine, ethynylenebis[diphenyl- Bis(diphenylphosphino)acetylene Phosphine, 1,2-ethynediylbis*diphenyl- Phosphine, ethynylenebis*diphenyl- ethynylenebis[diphenylphosphine]
Inchi:	InChI=1S/C26H20P2/c1-5-13-23(14-6-1)27(24-15-7-2-8-16-24)21-22-28(25-17-9-3-10-18
InchiKey:	FOWZHJNBFVLJGP-UHFFFAOYSA-N
Formula:	C26H20P2
SMILES:	C(#CP(c1ccccc1)c1ccccc1)P(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	394.38
CAS:	5112-95-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-17.16		Crippen Method
logp	5.171		Crippen Method
mcvol	314.480	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=C5112958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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