

Phosphorin, 2,4,6-tris(1,1-dimethylethyl)-

Inchi:	InChI=1S/C17H29P/c1-15(2,3)12-10-13(16(4,5)6)18-14(11-12)17(7,8)9/h10-11H,1-9H3
InchiKey:	GHJQOVICJOEYAD-UHFFFAOYSA-N
Formula:	C17H29P
SMILES:	CC(C)(C)c1cc(C(C)(C)C)pc(C(C)(C)C)c1
Mol. weight [g/mol]:	264.39
CAS:	17420-29-0

Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
log10ws	-2.41		Crippen Method
logp	6.159		Crippen Method
mcvol	247.090	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17420290&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

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

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