Diphosphene, bis(2,4,6-tri-tert-butylphenyl)-

Inchi: InChI=1S/C36H58P2/c1-31(2,3)23-19-25(33(7,8)9)29(26(20-23)34(10,11)12)37-38-30-27
InchiKey: JHIYGEOROKLMNN-UHFFFAOYSA-N
Formula: C36H58P2
SMILES: CC(C)(C)c1cc(C(C)(C)C)c(P=Pc2c(C(C)(C)C)cc(C(C)(C)C)cc2C(C)(C)C)c(C(C)(C)C)c1
Mol. weight [g/mol]: 552.79
CAS: 79073-99-7

Physical Properties

Property code	Value	Unit	Source
ie	6.80	eV	NIST Webbook
ie	7.24 ± 0.05	eV	NIST Webbook
ie	7.27	eV	NIST Webbook
log10ws	-13.29		Crippen Method
logp	11.230		Crippen Method
mcvol	507.200	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=C79073997&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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