

Phosphorin, 2,4,6-triphenyl-

Inchi: InChI=1S/C23H17P/c1-4-10-18(11-5-1)21-16-22(19-12-6-2-7-13-19)24-23(17-21)20-14-8
InchiKey: SPVWSVYJPGRPFL-UHFFFAOYSA-N
Formula: C23H17P
SMILES: c1ccc(-c2cc(-c3ccccc3)pc(-c3ccccc3)c2)cc1
Mol. weight [g/mol]: 324.35
CAS: 13497-36-4

Physical Properties

Property code	Value	Unit	Source
ie	7.80	eV	NIST Webbook
log10ws	-6.28		Crippen Method
logp	7.268		Crippen Method
mcvol	260.350	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13497364&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/25-293-9/Phosphorin-2-4-6-triphenyl.pdf>

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