((CH3)3C)(C6H5)2P=O

Other names: Phosphine oxide, (1,1-dimethylethyl)diphenyl-
tert-Butyldiphenylphosphine oxide
Phosphine oxide, tert-butyldiphenyl-
Phosphine oxide, t-butyldiphenyl-
t-C4H9(C6H5)2PO

Inchi: InChI=1S/C16H19OP/c1-16(2,3)18(17,14-10-6-4-7-11-14)15-12-8-5-9-13-15/h4-13H,1-3H

InchiKey: CHFOAXGMRFQIOK-UHFFFAOYSA-N

Formula: C16H19OP

SMILES: CC(C)(C)P(=O)(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 258.30

CAS: 56598-35-7

Physical Properties

Property code	Value	Unit	Source
affp	908.90	kJ/mol	NIST Webbook
basg	876.40	kJ/mol	NIST Webbook
log10ws	-13.90		Crippen Method
logp	3.799		Crippen Method
mcvol	215.110	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56598357&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

affp: Proton affinity

basg: Gas basicity

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume