

((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-C ₄ H ₉ (C ₆ H ₅) ₂ PO
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:	C ₁₆ H ₁₉ OP
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
mvol	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/ci9903071
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

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