

Phosphine oxide, t-butyldiphenyl-

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

Physical Properties

Property code	Value	Unit	Source
affp	908.90	kJ/mol	NIST Webbook
basg	876.40	kJ/mol	NIST Webbook
ie	8.28	eV	Cheméo Relay (1.0)
logp	3.799		Crippen Method
mcvol	215.110	ml/mol	McGowan Method
tf	423.27	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56598357&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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