# Phosphine oxide, t-butyldiphenyl-

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| **Other names:** | Phosphine oxide, (1,1-dimethylethyl)diphenyl-<br>tert-Butyldiphenylphosphine oxide<br>Phosphine oxide, tert-butyldiphenyl-<br>Phosphine oxide, t-butyldiphenyl-<br>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 |

## 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

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|---|---|
| **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/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |

## Legend

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