

Trimethylphosphine oxide

Other names: (CH₃)₃PO
Phosphine oxide, trimethyl-

Inchi: InChI=1S/C3H9OP/c1-5(2,3)4/h1-3H3

InchiKey: LRMLWYXJORUTBG-UHFFFAOYSA-N

Formula: C₃H₉OP

SMILES: CP(C)(C)=O

Mol. weight [g/mol]: 92.08

CAS: 676-96-0

Physical Properties

Property code	Value	Unit	Source
affp	909.70	kJ/mol	NIST Webbook
basg	880.00	kJ/mol	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.88	eV	NIST Webbook
ie	9.89	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.239		Crippen Method
mcvol	79.460	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C676960&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

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.cheméo.com/cid/77-920-5/Trimethylphosphine-oxide.pdf>

Generated by Cheméo on 2023-02-06 09:57:38.663018682 +0000 UTC m=+324694.253239195.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.