

Phosphine oxide, methyldiphenyl-

Other names:	(C6H5) ₂ (CH ₃)P=O CH ₃ (C ₆ H ₅) ₂ PO Diphenylmethylphosphine oxide Methyldiphenylphosphine oxide
Inchi:	InChI=1S/C13H13OP/c1-15(14,12-8-4-2-5-9-12)13-10-6-3-7-11-13/h2-11H,1H3
InchiKey:	PEGCITODQASXKH-UHFFFAOYSA-N
Formula:	C ₁₃ H ₁₃ OP
SMILES:	CP(=O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	216.22
CAS:	2129-89-7

Physical Properties

Property code	Value	Unit	Source
affp	908.90	kJ/mol	NIST Webbook
basg	876.40	kJ/mol	NIST Webbook
hfus	20.37	kJ/mol	Solubilities of Methyldiphenylphosphine Oxide in Selected Solvents
log10ws	-12.54		Crippen Method
logp	2.630		Crippen Method
mcvol	172.840	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.37	kJ/mol	385.40	NIST Webbook

Sources

Solubilities of Methyldiphenylphosphine Oxide in Selected Solvents:
McGowan Method:

<https://www.doi.org/10.1021/je900277m>

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2129897&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/48-264-6/Phosphine-oxide-methyldiphenyl.pdf>

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