

# Triphenylphosphine oxide

<b>Other names:</b>	(C6H5)3P=O (C6H5)3PO Triphenylphosphanoxid Triphenylphosphanoxide phosphine oxide, triphenyl- triphenyl phosphorus oxide triphenylphosphine monoxide
<b>Inchi:</b>	InChI=1S/C18H15OP/c19-20(16-10-4-1-5-11-16,17-12-6-2-7-13-17)18-14-8-3-9-15-18/h
<b>InchiKey:</b>	FIQMHBVFRAXMOP-UHFFFAOYSA-N
<b>Formula:</b>	C18H15OP
<b>SMILES:</b>	O=P(c1ccccc1)(c1ccccc1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	278.28
<b>CAS:</b>	791-28-6

## Physical Properties

Property code	Value	Unit	Source
affp	906.20	kJ/mol	NIST Webbook
basg	876.40	kJ/mol	NIST Webbook
hsub	66.00 ± 6.00	kJ/mol	NIST Webbook
log10ws	-18.12		Crippen Method
logp	3.326		Crippen Method
mcvol	219.530	ml/mol	McGowan Method
rinpol	2576.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tf	429.60 ± 0.30	K	NIST Webbook
tf	431.90 ± 0.50	K	NIST Webbook
tf	429.00 ± 1.00	K	NIST Webbook
tf	428.00 ± 4.00	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	339.00	J/molxK	314.00	NIST Webbook
cps	470.00	J/molxK	298.00	NIST Webbook

cps	317.00	J/mol×K	298.15	NIST Webbook
hfust	23.40	kJ/mol	429.60	NIST Webbook
hfust	24.22	kJ/mol	431.90	NIST Webbook
hfust	24.22	kJ/mol	431.90	NIST Webbook
hfust	24.22	kJ/mol	431.90	NIST Webbook
hfust	23.80	kJ/mol	429.00	NIST Webbook
hsubt	131.00 ± 2.00	kJ/mol	399.00	NIST Webbook
sfust	56.08	J/mol×K	431.90	NIST Webbook
sfust	95.60	J/mol×K	429.00	NIST Webbook

## Sources

Solubilities of Triphenylphosphine Oxide in Selected Solvents: McGowan Method:

<https://www.doi.org/10.1021/je800842z>

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C791286&Units=SI>

Crippen Method:

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

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>cps:</b>	Solid phase heat capacity
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>tf:</b>	Normal melting (fusion) point

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