Phosphine oxide, triphenyl-

Other names:	(C6H5)3P=O
	(C6H5)3PO
	Triphenylphosphanoxid
	Triphenylphosphanoxide
	triphenyl phosphorus oxide
	triphenylphosphine monoxide
	triphenylphosphine oxide
Inchi:	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/h1
InchiKey:	FIQMHBFVRAXMOP-UHFFFAOYSA-N
Formula:	C18H15OP
SMILES:	O=P(c1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	278.29

Physical Properties

Property code	Value	Unit	Source
af	0.5003		Cheméo Relay (1.0)
affp	906.20	kJ/mol	NIST Webbook
basg	876.40	kJ/mol	NIST Webbook
gf	249.89	kJ/mol	Cheméo Relay (1.0, beta)
hf	146.12	kJ/mol	Cheméo Relay (1.0)
hsub	66.00 ± 6.00	kJ/mol	NIST Webbook
hsub	66.00 ± 6.00	kJ/mol	NIST Webbook
hvap	105.55	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-4.60		Cheméo Relay (1.0)
logp	3.326		Crippen Method
mcvol	219.530	ml/mol	McGowan Method
pc	2268.49	kPa	Cheméo Relay (1.0, beta)
rinpol	2576.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	661.89	K	Cheméo Relay (1.0)
tc	934.49	K	Cheméo Relay (1.0)
tf	429.00 ± 1.00	K	NIST Webbook
tf	428.00 ± 4.00	K	NIST Webbook
tf	429.00 ± 1.00	K	NIST Webbook
tf	429.60 ± 0.30	K	NIST Webbook
tf	431.90 ± 0.50	K	NIST Webbook

vc	0.767	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	339.00	J/mol×K	314.00	NIST Webbook
cps	317.00	J/mol×K	298.15	NIST Webbook
cps	470.00	J/mol×K	298.00	NIST Webbook
hfust	24.22	kJ/mol	431.90	NIST Webbook
hfust	23.80	kJ/mol	429.00	NIST Webbook
hfust	23.80	kJ/mol	429.00	NIST Webbook
hfust	24.22	kJ/mol	431.90	NIST Webbook
hfust	24.22	kJ/mol	431.90	NIST Webbook
hfust	23.40	kJ/mol	429.60	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
sfust	95.60	J/mol×K	429.00	NIST Webbook

Sources

Solubilities of Triphenylphosphine Oxide in Selected Solvents: https://www.doi.org/10.1021/je800842z
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C791286&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

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
cps: Solid phase heat capacity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume