Phosphorus oxychloride

Other names:	Phosphoryl chloride
	Phosphoric chloride
	Phosphoric trichloride
	Phosphorus chloride oxide (POCl3)
	Phosphorus oxide trichloride
	Phosphorus oxytrichloride
	Phosphoryl trichloride
	Trichlorophosphine oxide
	Trichlorophosphorus oxide
	POCl3
	Phosphorus(V) trichloride oxide
	Phosphorous oxychloride
	Phosphorus oxide chloride
	Fosforoxychlorid
	Oxychlorid fosforecny
	UN 1810
	OPCl3
	Phosphoroxychloride
Inchi:	InChI=1S/Cl3OP/c1-5(2,3)4
InchiKey:	XHXFXVLFKHQFAL-UHFFFAOYSA-N
Formula:	Cl3OP
SMILES:	O=P(Cl)(Cl)Cl
Mol. weight [g/mol]:	153.33
CAS:	10025-87-3

Physical Properties

Property code	Value	Unit	Source
ea	1.41 ± 0.20	eV	NIST Webbook
ie	11.50 ± 0.10	eV	NIST Webbook
ie	11.36 ± 0.02	eV	NIST Webbook
ie	11.58 ± 0.05	eV	NIST Webbook
ie	11.40 ± 0.30	eV	NIST Webbook
ie	13.10 ± 0.20	eV	NIST Webbook
ie	11.89	eV	NIST Webbook
ie	11.89 ± 0.02	eV	NIST Webbook
ie	11.49	eV	NIST Webbook
ie	11.89 ± 0.03	eV	NIST Webbook

ie	12.00	eV	NIST Webbook
log10ws	-3.55		Crippen Method
logp	2.811		Crippen Method
mcvol	73.910	ml/mol	McGowan Method
pc	4960.00 ± 50.00	kPa	NIST Webbook
tc	601.00 ± 4.00	K	NIST Webbook
tf	274.35 ± 0.10	K	NIST Webbook
tf	274.20 ± 0.15	K	NIST Webbook
vc	0.276 ± 0.005	m3/kmol	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10025873&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

ea: Electron affinity

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume