

Phosphorus monoxide

Inchi:	InChI=1S/OP/c1-2
InchiKey:	LFGREXWGYUGZLY-UHFFFAOYSA-N
Formula:	OP
SMILES:	O=[P]
Mol. weight [g/mol]:	46.97
CAS:	14452-66-5

Physical Properties

Property code	Value	Unit	Source
affp	682.00	kJ/mol	NIST Webbook
basg	649.50	kJ/mol	NIST Webbook
ea	1.09 ± 0.01	eV	NIST Webbook
ea	1.00 ± 0.10	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
ie	8.90 ± 0.50	eV	NIST Webbook
ie	8.37	eV	NIST Webbook
ie	9.10 ± 0.50	eV	NIST Webbook
ie	8.39 ± 0.01	eV	NIST Webbook
ie	9.50 ± 0.50	eV	NIST Webbook
ie	9.00 ± 1.00	eV	NIST Webbook
ie	8.23	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
log10ws	-1.44		Crippen Method
logp	0.742		Crippen Method
mccvol	30.740	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14452665&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
ea:	Electron affinity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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