

Phosphoric Acid

Other names:	O-PHOSPHORIC ACID
Inchi:	InChI=1S/H3O4P/c1-5(2,3)4/h(H3,1,2,3,4)
InchiKey:	NBIIXXVUZAFBLC-UHFFFAOYSA-N
Formula:	H3O4P
SMILES:	O=P(O)(O)O
Mol. weight [g/mol]:	98.00
CAS:	7664-38-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	-0.929		Crippen Method
mcvol	54.800	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7664382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.chemeo.com/files/research/kdb/mol/mol1920.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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