phosphonic acid

Other names:	(HO)2HPO
	phosphorous acid
Inchi:	InChI=1S/H3O3P/c1-4(2)3/h4H,(H2,1,2,3)
InchiKey:	ABLZXFCXXLZCGV-UHFFFAOYSA-N
Formula:	H3O3P
SMILES:	O=[PH](O)O
Mol. weight [g/mol]:	82.00
CAS:	13598-36-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.81		Crippen Method
logp	-0.639		Crippen Method
mcvol	48.930	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13598362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic characteristics of reactions with KH(PO3H):	https://www.doi.org/10.1016/j.tca.2012.08.020
Densities, Viscosities, and Conductivities of Phosphonic Acid Solutions in N,N-Dimethylformamide and Water:	https://www.doi.org/10.1021/acs.jced.6b00430
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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