

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

Thermodynamic characteristics of reactions with KH(PO₃H): Densities, Viscosities, and Conductivities of Phosphonic Acid in Methanol, Dimethylformamide and Water:
NIST Webbook:

<https://www.doi.org/10.1016/j.tca.2012.08.020>

<https://www.doi.org/10.1021/acs.jced.6b00430>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13598362&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/10-280-9/phosphonic-acid.pdf>

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