

Methylphosphonic acid

Other names:	Methanephosphonic acid Phosphonic acid, methyl- p-methyl-phosphoric acid
Inchi:	InChI=1S/CH5O3P/c1-5(2,3)4/h1H3,(H2,2,3,4)
InchiKey:	YACKEPLHDIMKIO-UHFFFAOYSA-N
Formula:	CH5O3P
SMILES:	CP(=O)(O)O
Mol. weight [g/mol]:	96.02
CAS:	993-13-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.04		Crippen Method
logp	-0.206		Crippen Method
mcvol	63.020	ml/mol	McGowan Method
tf	382.11	K	Solubility of methylphosphonic acid in selected organic solvents

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of methylphosphonic acid in selected organic solvents:	https://www.doi.org/10.1016/j.fluid.2015.01.009
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C993135&Units=SI

Legend

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

tf: Normal melting (fusion) point

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