

Phosphonoacetic acid

Other names:	Acetic acid, phosphono- PPA Carboxymethanephosphonic acid Fosfonet Phosphonoacetic acid Fosfonoacetic acid
Inchi:	InChI=1S/C2H5O5P/c3-2(4)1-8(5,6)7/h1H2,(H,3,4)(H2,5,6,7)
InchiKey:	XUYJLQHKOGNDPB-UHFFFAOYSA-N
Formula:	C2H5O5P
SMILES:	O=C(O)CP(=O)(O)O
Mol. weight [g/mol]:	140.03
CAS:	4408-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.56		Crippen Method
logp	-0.751		Crippen Method
mcvol	84.550	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4408780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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