PHOSPHONOACETIC ACID

Other names:	Acetic acid, phosphono-
	PPA
	Carboxymethanephosphonic acid
	Fosfonet
	Phosphonacetic 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

Physical Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4408780&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume