Phosphonic acid, phenyl-

Other names:	Dihydrogen phenylphosphonate
	benzenephosphonic acid
	phenylphosphonic acid
	phosphonic acid, phenyl
Inchi:	InChI=1S/C6H7O3P/c7-10(8,9)6-4-2-1-3-5-6/h1-5H,(H2,7,8,9)
InchiKey:	QLZHNIAADXEJJP-UHFFFAOYSA-N
Formula:	C6H7O3P
SMILES:	O=P(O)(O)c1ccccc1
Mol. weight [g/mol]:	158.09
CAS:	1571-33-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	0.490		Crippen Method
mcvol	109.710	ml/mol	McGowan Method
tt	437.53	K	Solid-Liquid Equilibrium Solubility, Thermodynamic Properties, and Molecular Simulation of Phenylphosphonic Acid in 15 Pure Solvents at Different Temperatures

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid-Liquid Equilibrium Solubility, Thermodynamic Properties, and Molecular Simulation of Phenylphosphonic Acid in 15 Pure Solvents at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.9b00362
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1571331&Units=SI

Legend

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