

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

Solid-Liquid Equilibrium Solubility, Thermodynamic Properties, and McGowan Simulation of Phenylphosphonic Acid in 15 Pure Solvents at Different Temperatures:
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1571331&Units=SI>

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1021/acs.jced.9b00362>
<http://link.springer.com/article/10.1007/BF02311772>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

tt: Triple Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/73-079-4/Phosphonic-acid-phenyl.pdf>

Generated by Cheméo on 2024-04-09 17:40:34.729547437 +0000 UTC m=+14973683.650124811.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.