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

Physical Properties

Property code	Value	Unit	Source
ie	10.16	eV	Cheméo Relay (1.0)
logp	0.490		Crippen Method
mcvol	109.710	ml/mol	McGowan Method
tf	451.06	K	Cheméo Relay (1.0)
tt	437.53	K	Solid-Liquid Equilibrium Solubility, Thermodynamic Properties, and Molecular Simulation of Phenylphosphonic Acid in 15 Pure Solvents at Different Temperatures

Sources

Cheméo Relay (1.0, beta):

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1571331&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):

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature