

Phenylphosphonous acid

Other names:	Benzenephosphinic acid Benzenephosphonous acid Hydroxyphenylphosphine oxide Phenylphosphinic acid Phosphinic acid, phenyl-
Inchi:	InChI=1S/C6H7O2P/c7-9(8)6-4-2-1-3-5-6/h1-5,9H,(H,7,8)
InchiKey:	MLCHBQKMVKNBQV-UHFFFAOYSA-N
Formula:	C6H7O2P
SMILES:	O=[PH](O)c1ccccc1
Mol. weight [g/mol]:	142.09
CAS:	1779-48-2

Physical Properties

Property code	Value	Unit	Source
hfus	12.80	kJ/mol	Solubilities of Phenylphosphinic Acid, Methylphenylphosphinic Acid, Hexachlorocyclotriphosphazene, and Hexaphenoxycyclotriphosphazene in Selected Solvents
log10ws	-6.56		Crippen Method
logp	0.779		Crippen Method
mccvol	103.840	ml/mol	McGowan Method

Sources

Solubility of Phenylphosphinic Acid in Supercritical Carbon Dioxide and the Solubilities of Phenylphosphinic Acid, Hydroxymethylphenylphosphinic Acid, and Hexachlorocyclotriphosphazene, and Hexaphenoxycyclotriphosphazene in Selected Solvents:	https://www.doi.org/10.1021/acs.jced.9b00732
Crippen Method:	https://www.doi.org/10.1021/je050377q
McGowan Method:	https://www.doi.org/10.1021/je1009812
	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1779482&Units=SI
	http://pubs.acs.org/doi/abs/10.1021/ci990307l
	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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