

Phenylphosphine

Other names:	Phosphine, phenyl- Fenylfosfin
Inchi:	InChI=1S/C6H7P/c7-6-4-2-1-3-5-6/h1-5H,7H2
InchiKey:	RPGWZZNNEUHDAQ-UHFFFAOYSA-N
Formula:	C6H7P
SMILES:	Pc1ccccc1
Mol. weight [g/mol]:	110.09
CAS:	638-21-1

Physical Properties

Property code	Value	Unit	Source
ie	8.47 ± 0.01	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.187		Crippen Method
mcvol	92.100	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/33-922-1/Phenylphosphine.pdf>

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