

Phosphorodichloridous acid, phenyl ester

Other names:	Phenyl phosphorodichloridite phenyl dichlorophosphite
Inchi:	InChI=1S/C6H5Cl2OP/c7-10(8)9-6-4-2-1-3-5-6/h1-5H
InchiKey:	LXHWDUIRBUGRA-UHFFFAOYSA-N
Formula:	C6H5Cl2OP
SMILES:	<chem>CIP(Cl)Oc1ccccc1</chem>
Mol. weight [g/mol]:	194.98
CAS:	3426-89-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.30		Crippen Method
logp	3.770		Crippen Method
mcvol	122.450	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	52.70	kJ/mol	421.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3426899&Units=SI

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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