

Phosphorodichloridic acid, phenyl ester

Other names:	Dichlorophenoxyphosphine oxide NSC 44412 Phenoxydichlorophosphine oxide Phenoxyphosphoryl dichloride Phenyl dichlorophosphate Phenyl phosphorodichloridate Phenyl phosphorodichlorodate Phenylphosphoric dichloride Phosphoroyl dichloride phenyl ester
Inchi:	InChI=1S/C6H5Cl2O2P/c7-11(8,9)10-6-4-2-1-3-5-6/h1-5H
InchiKey:	TXFOLHZMICYNRM-UHFFFAOYSA-N
Formula:	C6H5Cl2O2P
SMILES:	O=P(Cl)(Cl)Oc1ccccc1
Mol. weight [g/mol]:	210.98
CAS:	770-12-7

Physical Properties

Property code	Value	Unit	Source
ie	9.10	eV	NIST Webbook
log10ws	-4.74		Crippen Method
logp	3.651		Crippen Method
mvol	128.320	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	63.60	kJ/mol	426.00	NIST Webbook

Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44423e+01
Coeff. B	-4.14629e+03
Coeff. C	-9.30900e+01
Temperature range (K), min.	386.02
Temperature range (K), max.	547.19

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C770127&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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

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