O-CHLOROPHENYL DICHLOROPHOSPHATE

Other names:	(2-Chlorophenyl)phosphoric acid dichloride
	2-Chlorophenyl phosphorodichloridate
	o-Chlorophenylphosphonyl dichloride
	Phosphorodichloridic acid, 2-chlorophenyl ester
	o-chlorophenyl dichlorophosphate
Inchi:	InChI=1S/C6H4Cl3O2P/c7-5-3-1-2-4-6(5)11-12(8,9)10/h1-4H
InchiKey:	VLDPXPPHXDGHEW-UHFFFAOYSA-N
Formula:	C6H4Cl3O2P
SMILES:	O=P(Cl)(Cl)Oc1ccccc1Cl
Mol. weight [g/mol]:	245.43

Physical Properties

Property code	Value	Unit	Source
hvap	65.85	kJ/mol	Cheméo Relay (1.0)
ie	9.29	eV	Cheméo Relay (1.0)
log10ws	-3.75		Cheméo Relay (1.0)
logp	4.304		Crippen Method
mcvol	140.560	ml/mol	McGowan Method
tb	510.86	K	Cheméo Relay (1.0)
tf	295.38	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15074541&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

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point