

t-Butyldichlorophosphine

Other names:	tert-C ₄ H ₉ PCl ₂ tert-Butyldichlorophosphine Phosponous dichloride, (1,1-dimethylethyl)-
Inchi:	InChI=1S/C ₄ H ₉ Cl ₂ P/c1-4(2,3)7(5)6/h1-3H3
InchiKey:	NMJASRUOIRRDSX-UHFFFAOYSA-N
Formula:	C ₄ H ₉ Cl ₂ P
SMILES:	CC(C)(C)P(Cl)Cl
Mol. weight [g/mol]:	158.99
CAS:	25979-07-1

Physical Properties

Property code	Value	Unit	Source
ie	9.00	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	0.25		Crippen Method
logp	3.574		Crippen Method
mcvol	112.160	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25979071&Units=SI
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

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/68-668-6/t-Butyldichlorophosphine.pdf>

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