

Methylphosphonyl dichloride

Other names:	Methyl phosphonic dichloride CH3POCl2 Methanephosphonic dichloride Methanephosphonic acid dichloride Phosphonic dichloride, methyl- NA 9206 Phosphonodichloridic acid, methyl- Methanephosphonyl chloride Phosphonic dichloride, P-methyl-
Inchi:	InChI=1S/CH3Cl2OP/c1-5(2,3)4/h1H3
InchiKey:	SCLFRABIDYGTAZ-UHFFFAOYSA-N
Formula:	CH3Cl2OP
SMILES:	CP(=O)(Cl)Cl
Mol. weight [g/mol]:	132.91
CAS:	676-97-1

Physical Properties

Property code	Value	Unit	Source
ie	11.40	eV	NIST Webbook
ie	10.91	eV	NIST Webbook
ie	10.92	eV	NIST Webbook
ie	11.49	eV	NIST Webbook
ie	11.45	eV	NIST Webbook
ie	11.43	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.287		Crippen Method
mcvol	75.760	ml/mol	McGowan Method
rinpol	802.00		NIST Webbook
rinpol	805.00		NIST Webbook
ss	164.84	J/mol×K	NIST Webbook
tt	306.14 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	131.12	J/mol×K	298.15	NIST Webbook
hfust	18.08	kJ/mol	306.14	NIST Webbook
hfust	18.08	kJ/mol	306.10	NIST Webbook
hfust	18.08	kJ/mol	306.10	NIST Webbook
sfust	59.04	J/mol×K	306.14	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C676971&Units=SI
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

Legend

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tt:	Triple Point Temperature

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