Methylphosphorodichloridate

Other names:	Methyl phosphorodichloridate
	Phosphorodichloridic acid, methyl ester
Inchi:	InChI=1S/CH3Cl2O2P/c1-5-6(2,3)4/h1H3
InchiKey:	SNVCRNWSNUUGEA-UHFFFAOYSA-N
Formula:	CH3Cl2O2P
SMILES:	COP(=O)(Cl)Cl
Mol. weight [g/mol]:	148.91

Physical Properties

Property code	Value	Unit	Source
hvap	42.30	kJ/mol	Cheméo Relay (1.0)
ie	11.50	eV	NIST Webbook
logp	2.218		Crippen Method
mcvol	81.630	ml/mol	McGowan Method
pc	4030.82	kPa	Cheméo Relay (1.0, beta)
tb	396.81	K	Cheméo Relay (1.0)
tc	595.31	K	Cheméo Relay (1.0)
tf	210.08	K	Cheméo Relay (1.0)
vc	0.320	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	331.50 ± 1.50	K	2.40	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C677247&Units=SI

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume