Phosphoric acid, trimethyl ester

Other names:	(CH3O)3PO
	Methyl phosphate
	Methyl phosphate, (MeO)3PO
	NCI-C03781
	NSC 58985
	O,O,O-Trimethyl phosphate
	TMP
	TMPA
	TMPO
	Trimethoxyphosphine oxide
	Trimethyl orthophosphate
	Trimethyl phosphate
	Trimethylfosfat
Inchi:	InChI=1S/C3H9O4P/c1-5-8(4,6-2)7-3/h1-3H3
InchiKey:	WVLBCYQITXONBZ-UHFFFAOYSA-N
Formula:	C3H9O4P
SMILES:	COP(=O)(OC)OC
Mol. weight [g/mol]:	140.07
CAS:	512-56-1

Physical Properties

Property code	Value	Unit	Source
affp	890.60	kJ/mol	NIST Webbook
basg	860.80	kJ/mol	NIST Webbook
hvap	47.50	kJ/mol	NIST Webbook
ie	10.77 ± 0.30	eV	NIST Webbook
ie	10.90	eV	NIST Webbook
ie	10.82	eV	NIST Webbook
ie	10.81	eV	NIST Webbook
ie	9.99	eV	NIST Webbook
ie	10.70 ± 0.10	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
log10ws	-1.60		Crippen Method
logp	1.034		Crippen Method
mcvol	97.070	ml/mol	McGowan Method
rinpol	902.00		NIST Webbook
rinpol	930.00		NIST Webbook

rinpol	932.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	921.00		NIST Webbook
tb	468.21	K	Estimation of Normal Boiling points of Trialkyl Phosphates using Retention indices by Gas Chromatography

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	47.50	kJ/mol	298.15	Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography
hvapt	48.80	kJ/mol	381.00	NIST Webbook
rhol	1217.10	kg/m3	293.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1212.90	kg/m3	298.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1207.80	kg/m3	303.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids

rhol	1202.50	kg/m3	308.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1198.00	kg/m3	313.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1191.90	kg/m3	318.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	1186.80	kg/m3	323.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54274e+01
Coeff. B	-4.76549e+03
Coeff. C	-2.92720e+01
Temperature range (K), min.	344.04
Temperature range (K), max.	500.36

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C512561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Towards understanding the effect of electrostatic interactions on the density of ionic liquids:	https://www.doi.org/10.1016/j.fluid.2009.02.011

Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.10.007
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Estimation of Normal Boiling points of Trialkyl Phosphates using Retention indices by Gas Chromatography:	https://www.doi.org/10.1016/j.tca.2010.07.032
Excess molar enthalpies for binary mixtures of trimethyl phosphate with alkanols {CH3(CH2)nOH, n= 0 3} at 298.15K:	https://www.doi.org/10.1016/j.tca.2008.02.015
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
hvap:	Enthalpy of vaporization at standard conditions
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature