

Triethyl phosphate

Other names: (C2H5O)3PO
Ethyl phosphate
Ethyl phosphate ((EtO)3PO)
Ethyl phosphate, tri-
NSC 2677
Phosphoric acid, triethyl ester
TEP
Triethoxyphosphine oxide
Triethylfosfat
Tris(ethyl) phosphate
o-Phosphoric acid triethyl ester

Inchi: InChI=1S/C6H15O4P/c1-4-8-11(7,9-5-2)10-6-3/h4-6H2,1-3H3
InchiKey: DQWPFSLDHJDLRL-UHFFFAOYSA-N
Formula: C6H15O4P
SMILES: CCOP(=O)(OCC)OCC
Mol. weight [g/mol]: 182.15
CAS: 78-40-0

Physical Properties

Property code	Value	Unit	Source
affp	909.30	kJ/mol	NIST Webbook
basg	879.60	kJ/mol	NIST Webbook
hvap	55.70	kJ/mol	NIST Webbook
ie	10.06 ± 0.27	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.79	eV	NIST Webbook
ie	12.80 ± 0.20	eV	NIST Webbook
ie	10.69	eV	NIST Webbook
ie	10.54	eV	NIST Webbook
ie	10.40	eV	NIST Webbook
log10ws	0.43		Aqueous Solubility Prediction Method
log10ws	0.43		Estimated Solubility Method
logp	2.204		Crippen Method
mcvol	139.340	ml/mol	McGowan Method
rinpol	1120.50		NIST Webbook

rinpol	1091.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1137.20		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1137.20		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1090.50		NIST Webbook
rinpol	1121.30		NIST Webbook
rinpol	1121.50		NIST Webbook
rinpol	1090.70		NIST Webbook
rinpol	1137.20		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1096.00		NIST Webbook
ripol	1672.10		NIST Webbook
ripol	1656.10		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1656.00		NIST Webbook
tb	489.00 ± 2.00	K	NIST Webbook
tb	489.04	K	Estimation of Normal Boiling points of Trialkyl Phosphates using Retention indices by Gas Chromatography
tf	216.95	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	55.73	kJ/mol	298.15	Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography
hvapt	46.30	kJ/mol	398.00	NIST Webbook

pvap	1.20e-03	kPa	271.25	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	1.24e-03	kPa	272.25	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	1.69e-03	kPa	275.25	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	2.22e-03	kPa	278.05	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
pvap	3.82e-03	kPa	283.15	Vapor Pressure of Triethyl and Tri-n-Propyl Phosphates and Diethyl Malonate
rhoI	1071.10	kg/m3	293.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	1067.90	kg/m3	298.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	1063.30	kg/m3	303.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	1058.90	kg/m3	308.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	1053.50	kg/m3	313.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids

rhoI	1048.00	kg/m3	318.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhoI	1043.20	kg/m3	323.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61069e+01
Coeff. B	-5.33572e+03
Coeff. C	-2.37130e+01
Temperature range (K), min.	361.00
Temperature range (K), max.	517.97

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78400&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Towards understanding the effect of electrostatic interactions on the density of ionic liquids:	https://www.doi.org/10.1016/j.fluid.2009.02.011
Estimation of Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Measurement of enthalpies of vaporization of trialkyl phosphates using Pressure-Temperature:	https://www.doi.org/10.1016/j.tca.2007.10.007
Tri-n-Propyl Phosphates and Diethyl Malonate:	https://www.doi.org/10.1021/je500428d
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
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
Relates the gas chromatography measurements of solubilities in ester absorbents for CO2 capture:	https://www.doi.org/10.1016/j.jct.2018.07.021

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
rho:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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