Tributyl phosphate

Other names:	Butyl phosphate
	Butyl phosphate, ((BuO)3PO)
	Butyl phosphate, tri-
	Celluphos 4
	Disflamoll TB
	Kronitex TBP
	NSC 8484
	Phosphoric acid tri-n-butyl ester
	Phosphoric acid tributyl ester
	Syn-O-Ad 8412
	TBP
	Tri-n-butyl phosphate
	Tributilfosfato
	Tributoxyphosphine oxide
	Tributyl ester of phosphoric acid
	Tributyle (phosphate de)
	Tributylfosfaat
	Tributylfosfat
	Tributylphosphat
	Tributylphsophate
	phosphoric acid, tributyl ester
	tributhyl phosphate
	tributoxy-hydroxyphosphanium
Inchi:	InChI=1S/C12H27O4P/c1-4-7-10-14-17(13,15-11-8-5-2)16-12-9-6-3/h4-12H2,1-3H3
InchiKey:	STCOOQWBFONSKY-UHFFFAOYSA-N
Formula:	C12H27O4P
SMILES:	CCCCOP(=O)(OCCCC)OCCCC
Mol. weight [g/mol]:	266.31
CAS:	126-73-8

Physical Properties

Property code	Value	Unit	Source
dvisc	0.0034500	Pa×s	Viscosity of the Tributyl Phosphate + Methyl Isobutyl Ketone + Phosphoric Acid System
hvap	81.30	kJ/mol	NIST Webbook

hvap	78.80	kJ/mol	NIST Webbook
hvap	81.70	kJ/mol	NIST Webbook
log10ws	-2.85		Aqueous Solubility Prediction Method
logp	4.545		Crippen Method
mcvol	223.880	ml/mol	McGowan Method
rinpol	1614.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	283.20		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	278.79		NIST Webbook
rinpol	283.20		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1638.70		NIST Webbook
rinpol	1647.40		NIST Webbook
rinpol	1647.90		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1615.70		NIST Webbook
rinpol	1658.80		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1615.00		NIST Webbook
ripol	2118.00		NIST Webbook

ripol	2075.00		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2157.40		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2114.20		NIST Webbook
ripol	2075.00		NIST Webbook
tb	561.34	K	Estimation of Normal Boiling points of Trialkyl Phosphates using Retention indices by Gas Chromatography
tf	193.48	K	Aqueous Solubility Prediction Method
tf	194.20	K	SLE and LLE for tri-butylphosphate or tri-octylamine contained systems; extractive solvents of Molybdenum
tf	194.31	K	Solid-Liquid Equilibria, Excess Molar Volumes, and Molar Refractivity Deviations for Extractive Solvents of Molybdenum

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	379.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0043040	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Tri-n-butyl Phosphate + Cyclohexane, + n-Heptane at T) (288.15, 293.15, 298.15, 303.15, and 308.15) K
dvisc	0.0020220	Pa×s	323.15	Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K

dvisc	0.0022200	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K
dvisc	0.0026510	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Tri-n-butyl Phosphate + Cyclohexane, + n-Heptane at T) (288.15, 293.15, 298.15, 303.15, and 308.15) K
dvisc	0.0029690	Pa×s	303.15	Densities and Viscosities of Binary Mixtures of Tri-n-butyl Phosphate + Cyclohexane, + n-Heptane at T) (288.15, 293.15, 298.15, 303.15, and 308.15) K
dvisc	0.0033410	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Tri-n-butyl Phosphate + Cyclohexane, + n-Heptane at T) (288.15, 293.15, 298.15, 303.15, and 308.15) K
dvisc	0.0018420	Pa×s	328.15	Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K
dvisc	0.0033990	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K

dvisc	0.0030120	Pa×s	303.15	Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K	
dvisc	0.0027020	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K	
dvisc	0.0024410	Pa×s	313.15	Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K	
dvisc	0.0037700	Pa×s	293.15	Densities and Viscosities of Binary Mixtures of Tri-n-butyl Phosphate + Cyclohexane, + n-Heptane at T) (288.15, 293.15, 298.15, 303.15, and 308.15) K	
hvapt	81.29	kJ/mol	298.15	Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography	
hvapt	61.40	kJ/mol	531.00	NIST Webbook	
rhol	976.00	kg/m3	293.15	Liquid-liquid equilibrium of 1-butanol + water +tri-n-butyl phosphate + ammonium chloride system	
rhol	959.93	kg/m3	313.15	Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate	

rhol	956.18	kg/m3	318.15	Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate
rhol	951.94	kg/m3	323.15	Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate
rhol	968.39	kg/m3	303.15	Density, Refractive Index, and Sound Velocity for the Binary Mixtures of Tri-n-Butyl Phosphate and n-Butanol between 303.15 K and 323.15 K
rhol	964.11	kg/m3	308.15	Density, Refractive Index, and Sound Velocity for the Binary Mixtures of Tri-n-Butyl Phosphate and n-Butanol between 303.15 K and 323.15 K
rhol	959.82	kg/m3	313.15	Density, Refractive Index, and Sound Velocity for the Binary Mixtures of Tri-n-Butyl Phosphate and n-Butanol between 303.15 K and 323.15 K
rhol	964.60	kg/m3	293.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	961.60	kg/m3	298.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids

rhol	958.40	kg/m3	303.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	955.40	kg/m3	308.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	949.60	kg/m3	313.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	944.70	kg/m3	318.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	940.90	kg/m3	323.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
rhol	972.69	kg/m3	298.15	Liquid-liquid equilibria for aqueous sulfuric acid solutions with undecane, dodecane, or 1-dodecanol, trioctylamine or tributyl phosphate and excess and deviation properties for sub-binary systems at 298.15 K
rhol	972.69	kg/m3	298.15	Liquid-liquid equilibria, excess molar volume and deviations of the refractive indices at 298.15 K for mixtures of solvents used in themolybdenum extraction process

rhol	955.54	kg/m3	318.15	Density, Refractive Index, and Sound Velocity for the Binary Mixtures of Tri-n-Butyl Phosphate and n-Butanol between 303.15 K and 323.15 K	
rhol	972.70	kg/m3	293.20	Modeling extraction equilibria of butyric acid distributed between water and tri-n-butyl amine/diluent or tri-n-butyl phosphate/diluent system: Extension of the LSER approach	
rhol	973.85	kg/m3	298.15	Volumetric and acoustic properties of binary mixtures of tri-n-butyl phosphate with n-hexane, cyclohexane, and n-heptane from T = (298.15 to 323.15) K	
rhol	969.44	kg/m3	303.15	Volumetric and acoustic properties of binary mixtures of tri-n-butyl phosphate with n-hexane, cyclohexane, and n-heptane from T = (298.15 to 323.15) K	
rhol	965.04	kg/m3	308.15	Volumetric and acoustic properties of binary mixtures of tri-n-butyl phosphate with n-hexane, cyclohexane, and n-heptane from T = (298.15 to 323.15) K	

rhol	960.62	kg/m3	313.15	Volumetric and acoustic properties of binary mixtures of tri-n-butyl phosphate with n-hexane, cyclohexane, and n-heptane from T = (298.15 to 323.15) K
rhol	956.19	kg/m3	318.15	Volumetric and acoustic properties of binary mixtures of tri-n-butyl phosphate with n-hexane, cyclohexane, and n-heptane from T = (298.15 to 323.15) K
rhol	951.75	kg/m3	323.15	Volumetric and acoustic properties of binary mixtures of tri-n-butyl phosphate with n-hexane, cyclohexane, and n-heptane from T = (298.15 to 323.15) K
rhol	972.77	kg/m3	298.15	Volumetric and compressibility studies on tri-n-butyl phosphate (TBP)-phase modifier (1-octanol, 1-decanol and isodecanol) interactions from T = (298.15 to 323.15) K
rhol	968.46	kg/m3	303.15	Volumetric and compressibility studies on tri-n-butyl phosphate (TBP)-phase modifier (1-octanol, 1-decanol and isodecanol) interactions from T = (298.15 to 323.15) K

rhol	964.15	kg/m3	308.15	Volumetric and compressibility studies on tri-n-butyl phosphate (TBP)-phase modifier (1-octanol, 1-decanol and isodecanol) interactions from T = (298.15 to 323.15) K	
rhol	959.84	kg/m3	313.15	Volumetric and compressibility studies on tri-n-butyl phosphate (TBP)-phase modifier (1-octanol, 1-decanol and isodecanol) interactions from T = (298.15 to 323.15) K	
rhol	955.52	kg/m3	318.15	Volumetric and compressibility studies on tri-n-butyl phosphate (TBP)-phase modifier (1-octanol, 1-decanol and isodecanol) interactions from T = (298.15 to 323.15) K	
rhol	951.20	kg/m3	323.15	Volumetric and compressibility studies on tri-n-butyl phosphate (TBP)-phase modifier (1-octanol, 1-decanol and isodecanol) interactions from T = (298.15 to 323.15) K	
rhol	972.82	kg/m3	298.15	Thermodynamics of mixing for binary mixtures of 1-octanol and 1-decanol with n-dodecane and ternary mixture of (TBP + 1-octanol + dodecane) at T = (298.15 to 323.15) K	

rhol	968.50	kg/m3	303.15	Thermodynamics of mixing for binary mixtures of 1-octanol and 1-decanol with n-dodecane and ternary mixture of (TBP + 1-octanol + dodecane) at T = (298.15 to 323.15) K
rhol	964.18	kg/m3	308.15	Thermodynamics of mixing for binary mixtures of 1-octanol and 1-decanol with n-dodecane and ternary mixture of (TBP + 1-octanol + dodecane) at T = (298.15 to 323.15) K
rhol	959.86	kg/m3	313.15	Thermodynamics of mixing for binary mixtures of 1-octanol and 1-decanol with n-dodecane and ternary mixture of (TBP + 1-octanol + dodecane) at T = (298.15 to 323.15) K
rhol	955.53	kg/m3	318.15	Thermodynamics of mixing for binary mixtures of 1-octanol and 1-decanol with n-dodecane and ternary mixture of (TBP + 1-octanol + dodecane) at T = (298.15 to 323.15) K
rhol	951.20	kg/m3	323.15	Thermodynamics of mixing for binary mixtures of 1-octanol and 1-decanol with n-dodecane and ternary mixture of (TBP + 1-octanol + dodecane) at T = (298.15 to 323.15) K
rhol	976.92	kg/m3	293.15	Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate

rhol	972.79	kg/m3	298.15	Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate
rhol	968.59	kg/m3	303.15	Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate
rhol	964.16	kg/m3	308.15	Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate
rhol	951.26	kg/m3	323.15	Density, Refractive Index, and Sound Velocity for the Binary Mixtures of Tri-n-Butyl Phosphate and n-Butanol between 303.15 K and 323.15 K
srf	0.03	N/m	323.15	Surface tension of binary mixtures of (ionic liquid + tributyl phosphate)
srf	0.03	N/m	318.15	Surface tension of binary mixtures of (ionic liquid + tributyl phosphate)
srf	0.03	N/m	313.15	Surface tension of binary mixtures of (ionic liquid + tributyl phosphate)
srf	0.03	N/m	308.15	Surface tension of binary mixtures of (ionic liquid + tributyl phosphate)
srf	0.03	N/m	303.15	Surface tension of binary mixtures of (ionic liquid + tributyl phosphate)

srf	0.03	N/m	298.15	Surface tension of binary mixtures of (ionic liquid + tributyl phosphate)
srf	0.03	N/m	293.15	Surface tension of binary mixtures of (ionic liquid + tributyl phosphate)

Sources

Liquid-liquid equilibrium of 1-butanol + water +tri-n-butyl phosphate + ammonium chloride system:	https://www.doi.org/10.1016/j.fluid.2014.06.023
Towards understanding the effect of electrostatic interactions on the density of ionic liquids:	https://www.doi.org/10.1016/j.fluid.2009.02.011
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solid-Liquid Equilibria, Excess Molar Volumes, and Molar Refractivity Deviations for Extractive Solvents of Molybdenum:	https://www.doi.org/10.1021/je900586f
Surface tension of binary mixtures of (ionic liquid + tributyl phosphate):	https://www.doi.org/10.1016/j.jct.2018.12.036
Volumetric and acoustic properties of binary mixtures of tri-n-butyl phosphate with n-hexane, cyclohexane, and n-heptane from T = (298.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2012.09.015
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126738&Units=SI
Thermodynamics of mixing for binary mixtures of 1-octanol and 1-decanol with n-dodecane and ternary mixture of (TBP + 1-octanol + dodecane) at T = (298.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2015.06.029
SLE and LLE for tri-butylphosphate or trioctylamine contained systems:	https://www.doi.org/10.1016/j.fluid.2010.04.016
Density, Refractive Index, and Sound Velocity for the Binary Mixtures of Tri-n-Butyl Phosphate and n-Butanol between 303.15 K and 323.15 K:	https://www.doi.org/10.1021/acs.jced.5b00343
Solubility Measurement and Thermodynamic Modeling of Benzoic Acid in Monosolvents and Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.8b00025
Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.10.007
Solubilities of sulfuryl fluoride in propylene carbonate, tributyl phosphate and N-methylpyrrolidone:	https://www.doi.org/10.1016/j.jct.2018.05.007
Liquid-liquid equilibria, excess molar volume and deviations of the refractive indices at 298.15 K for mixtures of solvents used in the molybdenum extraction process:	https://www.doi.org/10.1016/j.fluid.2013.06.013
Below the room temperature measurements of solubilities in ester absorbents for CO2 capture:	https://www.doi.org/10.1016/j.jct.2018.07.021
Densities and Viscosities of Binary Mixtures of Tri-n-butyl Phosphate + Cyclohexane, + n-Heptane at T = (288.15, 293.15, 298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je8003707
Liquid Liquid Equilibria for the Quaternary System H3PO4-NaCl-H2O-TBP at 298.15 K:	https://www.doi.org/10.1021/je400817m
Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate:	https://www.doi.org/10.1016/j.jct.2018.04.005
Volumetric and compressibility studies on tri-n-butyl phosphate (TBP)-phase modifier (1-octanol, 1-decanol and isodecanol) interactions from T = (298.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2013.10.018
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
Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K:	https://www.doi.org/10.1021/je060491o
Liquid-liquid equilibria for aqueous sulfuric acid solutions with undecane, dodecane, or 1-dodecanol, trioctylamine or tributyl phosphate and excess and deviation properties for sub-binary systems at 298.15 K:	https://www.doi.org/10.1016/j.fluid.2013.01.002
Viscosity of the Tributyl Phosphate + Methyl Isobutyl Ketone + Phosphoric Acid System:	https://www.doi.org/10.1021/je700746a
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous/Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335
Thermodynamic Properties and Phase Equilibria in the Water-Tri-n-butyl Phosphate System:	https://www.doi.org/10.1021/acs.jced.6b00582
Molar excess enthalpies of binary mixtures of [tributyl phosphate + {CH3(CH2)nOH (n = 0 to 5)}] at 298.15 K:	https://www.doi.org/10.1016/j.jct.2006.08.001
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Liquid-Liquid Equilibrium in the System Phosphoric Acid/Water/Tri-n-butyl Phosphate/Calcium Chloride:	https://www.doi.org/10.1021/je100054k
Modeling extraction equilibria of butyric acid distributed between water and tri-n-butyl amine/diluent or tri-n-butyl phosphate/diluent system: Extension of the LSER approach:	https://www.doi.org/10.1016/j.fluid.2014.10.043

Legend

cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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