Tri-n-butylphosphate

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
	Tributilfosfato
	Tributyl ester of phosphoric acid
	Tributyle (phosphate de)
	Tributylfosfaat
	Tributylfosfat
	Tributylphosphat
	Tributylphsophate
	phosphoric acid, tributyl ester
	tri-n-butyl phosphate
	tributhyl phosphate
	tributoxy-hydroxyphosphanium
	tributoxyphosphine oxide
	tributyl phosphate
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]:	266.32

Physical Properties

Property code	Value	Unit	Source
af	0.7347		Cheméo Relay (1.0)
dvisc	0.0034500	Pa×s	Viscosity of the Tributyl Phosphate + Methyl Isobutyl Ketone + Phosphoric Acid System

gf	-411.12	kJ/mol	Cheméo Relay (1.0, beta)
hf	-972.68	kJ/mol	Cheméo Relay (1.0)
hvap	81.30	kJ/mol	NIST Webbook
hvap	81.70	kJ/mol	NIST Webbook
hvap	78.80	kJ/mol	NIST Webbook
ie	10.20	eV	Cheméo Relay (1.0)
log10ws	-2.85		Aqueous Solubility Prediction Method
logp	4.545		Crippen Method
mcvol	223.880	ml/mol	McGowan Method
pc	1776.19	kPa	Cheméo Relay (1.0, beta)
rinpol	1623.00		NIST Webbook
rinpol	283.20		NIST Webbook
rinpol	1615.70		NIST Webbook
rinpol	1658.80		NIST Webbook
rinpol	1613.00		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	1614.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	278.79		NIST Webbook
rinpol	283.20		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1623.00		NIST Webbook
rinpol	1647.90		NIST Webbook
rinpol	1647.40		NIST Webbook
rinpol	1638.70		NIST Webbook
rinpol	1616.00		NIST Webbook

rinpol	1663.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1613.00		NIST Webbook
ripol	2114.20		NIST Webbook
ripol	2075.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2075.00		NIST Webbook
ripol	2157.40		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2079.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2079.00		NIST Webbook
tb	561.34	K	Estimation of Normal Boiling points of Trialkyl Phosphates using Retention indices by Gas Chromatography
tc	691.02	K	Cheméo Relay (1.0)
tf	193.48	K	Aqueous Solubility Prediction Method
tf	194.31	K	Solid-Liquid Equilibria, Excess Molar Volumes, and Molar Refractivity Deviations for Extractive Solvents of Molybdenum
tf	194.20	K	SLE and LLE for tri-butylphosphate or tri-octylamine contained systems; extractive solvents of Molybdenum
vc	0.870	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	379.40	J/mol×K	298.15	NIST Webbook
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

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	0.0024410	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	0.0022200	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	0.0030120	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	0.0026510	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	0.0027020	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	0.0033990	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	0.0043040	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	0.0018420	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	0.0020220	Pa×s	323.15	Densities and Viscosities of Binary Mixtures of Tributyl Phosphate with Hexane and Dodecane from (298.15 to 328.15) K
hvapt	61.40	kJ/mol	531.00	NIST Webbook
hvapt	81.29	kJ/mol	298.15	Measurement of enthalpies of vaporization of trialkyl phosphates using correlation gas chromatography

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	959.93	kg/m3	313.15	Volumetric properties of binary mixtures of ionic liquid with tributyl phosphate and dimethyl carbonate	
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	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	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	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	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	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	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
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	976.00	kg/m3	293.15	Liquid-liquid equilibrium of 1-butanol + water +tri-n-butyl phosphate + ammonium chloride system
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	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	940.90	kg/m3	323.15	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	949.60	kg/m3	313.15	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	958.40	kg/m3	303.15	Towards understanding the effect of electrostatic interactions on the density of ionic liquids
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)

srf	0.03	N/m	303.15	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	313.15	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	323.15	Surface tension of binary mixtures of (ionic liquid + tributyl phosphate)

Sources

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
Modeling extraction equilibria of butyric acid distributed between water and tri-n-butylamine/diluent or tri-n-butyl phosphate/diluent system: Extension of the LSER approach:	https://www.doi.org/10.1016/j.fluid.2014.10.043
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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Solid-Liquid Equilibria, Excess Molar Volumes, and Molar Refractivity Deviations for Extractive Solvents of Molybdenum:	https://www.doi.org/10.1021/je900586f
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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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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
Below the room temperature measurements of solubilities in ester absorbents for CO2 capture:	https://www.doi.org/10.1016/j.jct.2018.07.021
Solubility Measurement and Thermodynamic Modeling of Benzoic Acid in Monosolvents and Binary Mixtures:	https://www.doi.org/10.1021/acs.jced.8b00025
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
Solubilities of sulfuryl fluoride in propylene carbonate, tributyl phosphate and N-methylpyrrolidone:	https://www.doi.org/10.1016/j.jct.2018.05.007
Towards understanding the effect of electrostatic interactions on the density of ionic liquids:	https://www.doi.org/10.1016/j.fluid.2009.02.011
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
Volumetric and compressibility studies on tri-n-butyl phosphate (TBP)-phase modifier (1-decanol and isodecanol) interactions from T = (298.15 to 323.15) K:	https://www.doi.org/10.1016/j.jct.2013.10.018
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
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
SLE and LLE for tri-butylphosphate or tri-octylamine contained systems; extractive solvents of Molybdenum:	https://www.doi.org/10.1016/j.fluid.2010.04.016
Surface tension of binary mixtures of (ionic liquid + tributyl phosphate):	https://www.doi.org/10.1016/j.jct.2018.12.036

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Molar excess enthalpies of binary mixtures of tributyl phosphate + n-octylamine or tributyl phosphate + Phosphoric Acid/Water/(1:1 n-butyl Phosphate:Dodecan-1-ol): https://www.doi.org/10.1016/j.jct.2006.08.001

Liquid-Liquid Equilibrium in the System Water + Phosphoric Acid + Tributyl Phosphate at 298.15 K: https://www.doi.org/10.1021/je100054k

Excess and solution properties of ternary systems containing tributyl phosphate + dodecane + 1-dodecanol at 298.15 K: https://www.doi.org/10.1016/j.tca.2007.10.007

Molar excess enthalpies of binary mixtures of tributyl phosphate + cyclohexane and + heptane from (298.15 to 328.15) K: https://www.doi.org/10.1016/j.jct.2012.09.015

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HoPO4-NaCl-H2O-TBP at 298.15 K:

vaporization of trialkyl phosphates using correlation gas chromatography: http://link.springer.com/article/10.1007/BF02311772

McGowan Method:

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Estimation of Normal Boiling points of Trialkyl Phosphates using Retention Indices Determined by Gas Chromatography: https://www.doi.org/10.1021/je400817m

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C126738&Units=SI

Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume