

Tetrabutylphosphonium bromide

Other names:	Phosphonium bromide, tetrabutyl Phosphonium, tetrabutyl-, bromide Tertabutylphosphoriun bromide tetra-n-Butylphosphonium bromide
Inchi:	InChI=1S/C16H36BrP/c1-5-9-13-18(17,14-10-6-2,15-11-7-3)16-12-8-4/h5-16H2,1-4H3
InchiKey:	ZTGKRWWWUGCLHZ-UHFFFAOYSA-N
Formula:	C16H36BrP
SMILES:	CCCCP(Br)(CCCC)(CCCC)CCCC
Mol. weight [g/mol]:	339.33
CAS:	3115-68-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	7.050		Crippen Method
mcvol	278.560	ml/mol	McGowan Method

Sources

Extraction of caffeine using aqueous two-phase systems containing ionic liquids and ionic liquids, and	https://www.doi.org/10.1016/j.fluid.2019.112287
Densities, Viscosities, and Conductivities of Aqueous Solutions of Tetra-n-butylphosphonium Bromide and Ethyltributylphosphonium Bromide at Different Temperatures	https://www.doi.org/10.1021/je400101s
Efficient separation of curcumin using tetra butyl phosphonium bromide / Efficient and Reversible Nitric Oxide Absorption by Ionic Liquids	https://www.chemeo.com/doc/models/crippen_log10ws
Aqueous Two-Phase Systems: Aqueous Two-Phase Systems: Aqueous Two-Phase Systems	https://www.doi.org/10.1016/j.fluid.2019.06.015
Compressibility of Tetrabutylphosphonium Bromide in Various Solvents	https://www.doi.org/10.1021/acs.jced.9b00173
Phase diagrams of ionic liquids-based aqueous biphasic systems as a function of extraction processes:	https://www.doi.org/10.1021/je900888e
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	https://www.doi.org/10.1016/j.jct.2013.10.024
	http://pubs.acs.org/doi/abs/10.1021/ci9903071
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3115682&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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