Methyltriphenylphosphonium bromide

Other names:	Phosphonium, methyltriphenyl-, bromide
	Triphenylmethylphosphonium bromide
Inchi:	InChI=1S/C19H18BrP/c1-21(20,17-11-5-2-6-12-17,18-13-7-3-8-14-18)19-15-9-4-10-16-1
InchiKey:	BKRKYEFQSANYGA-UHFFFAOYSA-N
Formula:	C19H18BrP
SMILES:	CP(Br)(c1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	357.22
CAS:	1779-49-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.64		Crippen Method
logp	4.456		Crippen Method
mcvol	249.550	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Application of the Eotvos and Guggenheim empirical rules for predicting the density and surface tension of ionic liquids analogues:	https://www.doi.org/10.1016/j.tca.2013.10.017
Prediction of refractive index and density of deep eutectic solvents using atomic contributions:	https://www.doi.org/10.1016/j.fluid.2013.06.050
Electrical conductivity of ammonium and phosphonium based deepeutectic solvents: Measurements and artificial intelligence basedprediction:	https://www.doi.org/10.1016/j.fluid.2013.07.012
Preparation and characterization of amine (N methyl diethanolamine) based transition temperature mixtures (deep eutectic analogues solvents):	https://www.doi.org/10.1016/j.jct.2018.12.014
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1779493&Units=SI
Oil desulfurization using deep eutectic solvents as sustainable and economical extractants via liquid-liquid extraction: Experimental and PC-SAFT predictions:	https://www.doi.org/10.1016/j.fluid.2018.03.018
Molar Heat Capacity of Selected Type III Deep Eutectic Solvents. Phosphonium-Based Ionic Liquids Analogues and Their Physical Properties:	https://www.doi.org/10.1021/acs.jced.5b00989
Densities of Ammonium and Phosphonium based Deep Eutectic Solvents: Prediction using Artificial Intelligence and Group Contribution Techniques:	https://www.doi.org/10.1021/je100104v
Monoethanolamine-based deep eutectic solvents, their synthesis and characterisation:	https://www.doi.org/10.1016/j.tca.2011.10.010
Liquid-Liquid Equilibrium Measurements for the Extraction of Pyridine and Benzothiazole from n-Alkanes Using Deep Eutectic Solvents:	https://www.doi.org/10.1016/j.fluid.2017.03.008
Effect of the Type of Ammonium Salt on the Extractive Desulfurization of Fuels Using Deep Eutectic Solvents:	https://www.doi.org/10.1021/acs.jced.9b00413
	https://www.doi.org/10.1021/acs.jced.7b00832

Legend

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