TETRABUTYLAMMONIUM HEXAFLUOROPHOSPHATE

Other names: 1-Butanaminium, N,N,N-tributyl-, hexafluorophosphate(1-)

Inchi: InChI=1S/C16H36N.F6P/c1-5-9-13-17(14-10-6-2,15-11-7-3)16-12-8-4;1-7(2,3,4,5)6/h5-1

InchiKey: BKBKEFQIOUYLBC-UHFFFAOYSA-N

Formula: C16H36F6NP

SMILES: CCCC[N+](CCCC)(CCCC)CCCC.F[P-](F)(F)(F)(F)F

Mol. weight [g/mol]: 387.43

Physical Properties

Property code	Value	Unit	Source
af	0.6316		Cheméo Relay (1.0)
gf	-1116.30	kJ/mol	Cheméo Relay (1.0, beta)
hf	-2157.39	kJ/mol	Cheméo Relay (1.0)
hvap	48.73	kJ/mol	Cheméo Relay (1.0)
ie	12.47	eV	Cheméo Relay (1.0)
log10ws	-5.01		Cheméo Relay (1.0)
pc	702.47	kPa	Cheméo Relay (1.0, beta)
tb	520.80	K	Cheméo Relay (1.0)
tc	512.95	K	Cheméo Relay (1.0)
tf	524.30	K	Solubility of non-aromatic hexafluorophosphate-based salts and ionic liquids in water determined by electrical conductivity
tf	517.20 ± 0.50	K	NIST Webbook
tf	344.15	K	Ion exchange synthesis and thermal characteristics of some [N+ 4444] based ionic liquids
vc	0.938	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Ionic solvation of tetrabutylammonium hexafluorophosphate in pure nitromethane, 1, 3-dioxolane and nitrobenzene: A comparative physicochemical study: https://www.doi.org/10.1016/j.fluid.2011.11.002

Solubility of non-aromatic hexafluorophosphate-based salts and ionic liquids in water determined by electrical conductivity: https://www.doi.org/10.1016/j.fluid.2013.07.061

Volumetric and compressibility behaviour of ionic liquid, 1-n-butyl-3-methylimidazolium hexafluorophosphate and tetrabutylammonium hexafluorophosphate in organic solvents at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.07.018
Ion exchange synthesis and thermal characteristics of some [N+ 4444] salts of [PF6]- and [BF4]- anions	https://www.doi.org/10.1016/j.tca.2013.01.003
NIST Webbook: Tetrabutylammonium hexafluorophosphate	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3109635&Units=SI

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume