

1-Ethylpyridinium bromide

Other names:	Ethyl pyridinium bromide Pyridinium, 1-ethyl-, bromide
Inchi:	InChI=1S/C7H10BrN/c1-2-9(8)6-4-3-5-7-9/h3-7H,2H2,1H3
InchiKey:	VGFAPFPMWQYBIW-UHFFFAOYSA-N
Formula:	C7H10BrN
SMILES:	CC[N+](Br)C=CC=C[CH-]1
Mol. weight [g/mol]:	188.06
CAS:	1906-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	2.378		Crippen Method
mcvol	117.510	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Great increase of the electrical conductivity of ionic liquids in aqueous two-phase systems of the ionic liquid bromate in the presence of an aqueous solution of propylate sodium sulfate	https://www.doi.org/10.1016/j.fluid.2006.05.028
Equilibrium liquid-liquid equilibria of an ionic liquid in the presence of an aqueous solution of propylate sodium sulfate	https://www.doi.org/10.1016/j.fluid.2012.12.019
McGowan's method for the determination of logp and log10ws and correlations and application to temperatures	https://www.doi.org/10.1016/j.fluid.2019.05.003
Experimental determination and correlation:	http://link.springer.com/article/10.1007/BF02311772 http://webbook.nist.gov/cgi/cbook.cgi?ID=C1906792&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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