Pyridinium, 1-[(hydroxyphenylmethylene)amino]-2-methyl-, hydroxide, inner salt

Other names:	2-Picolinium, 1-[(«alpha»-hydroxybenzylidene)amino]-, hydroxide, inner salt
	Pyridinium, 1-(benzoylamino)-2-methyl-, hydroxide, inner salt
	2-Picolinium, 1-benzamido-, hydroxide, inner salt
Inchi:	InChI=1S/C13H12N2O/c1-11-7-5-6-10-15(11)14-13(16)12-8-3-2-4-9-12/h2-10H,1H3
InchiKey:	CDHJGSMLGXTKDG-UHFFFAOYSA-N
Formula:	C13H12N2O
SMILES:	Cc1cccc[n+]1[N-]C(=O)c1ccccc1
Mol. weight [g/mol]:	212.25
CAS:	17408-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.56		Crippen Method
logp	2.260		Crippen Method
mcvol	168.040	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17408478&Units=SI

Legend

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