Pyridinium, 1-(benzoylamino)-4-methyl-, hydroxide, inner salt

Other names: 4-Picolinium, 1-benzamido-, hydroxide, inner salt
N-Benzoylimino-4-methylpyridinium betaine

Inchi: InChI=1S/C13H12N2O/c1-11-7-9-15(10-8-11)14-13(16)12-5-3-2-4-6-12/h2-10H,1H3

InchiKey: BKCJEFFBFUEEQD-UHFFFAOYSA-N

Formula: C13H12N2O

SMILES: Cc1cc[n+]([N-]C(=O)c2ccccc2)cc1

Mol. weight [g/mol]: 212.25

CAS: 32363-75-0

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=C32363750&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.