

1-[(4-Bromophenyl)methyl]pyridinium

Inchi:	InChI=1S/C12H11BrN/c13-12-6-4-11(5-7-12)10-14-8-2-1-3-9-14/h1-9H,10H2/q+1
InchiKey:	LADMUUSDJBIFDI-UHFFFAOYSA-N
Formula:	C12H11BrN
SMILES:	<chem>Brc1ccc(C[n+]2ccccc2)cc1</chem>
Mol. weight [g/mol]:	249.13
CAS:	89047-29-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	2.785		Crippen Method
mcvol	162.050	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89047290&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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<https://www.chemeo.com/cid/68-006-0/1-4-Bromophenyl-methyl-pyridinium.pdf>

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