1[(4-Chlorophenyl)methyl]pyridinium

Inchi: InChI=1S/C12H11ClN/c13-12-6-4-11(5-7-12)10-14-8-2-1-3-9-14/h1-9H,10H2/q+1
InchiKey: GDGNYUXBILMTKL-UHFFFAOYSA-N
Formula: C12H11ClN
SMILES: Clc1ccc(C[n+]2ccccc2)cc1
Mol. weight [g/mol]: 204.68
CAS: 71897-27-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.15		Crippen Method
logp	2.676		Crippen Method
mcvol	156.790	ml/mol	McGowan Method

Sources

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=C71897273&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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