1-[(Phenylthio)methyl]pyridinium

Inchi: InChI=1S/C12H12NS/c1-3-7-12(8-4-1)14-11-13-9-5-2-6-10-13/h1-10H,11H2/q+1
InchiKey: LHMRTNGWGSTIGK-UHFFFAOYSA-N
Formula: C12H12NS
SMILES: c1ccc(SC[n+]2ccccc2)cc1
Mol. weight [g/mol]: 202.29
CAS: 71880-02-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.22		Crippen Method
logp	2.724		Crippen Method
mcvol	160.900	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=C71880029&Units=SI

Legend

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