

Isoxazolium compounds: 2-ethyl-5-(m-sulfophenyl)-hydroxide, inner salt

InChI:	InChI=1S/C11H11NO4S/c1-2-12-7-10(8-16-12)9-4-3-5-11(6-9)17(13,14)15/h3-8H,2H2,1H
InChIKey:	VRTQQJBZFOSHCJ-UHFFFAOYSA-N
Formula:	C11H11NO4S
SMILES:	CC[n+]1cc(-c2cccc(S(=O)(=O)[O-])c2)co1
Mol. weight [g/mol]:	253.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.42		Crippen Method
logp	1.158		Crippen Method
mcvol	172.440	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=B6007190&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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