Benzenaminium, 2-hydroxy-N,N,N-trimethyl-, hydroxide, inner salt

Other names: Ammonium, (o-hydroxyphenyl)trimethyl-, hydroxide, inner salt
Inchi: InChI=1S/C9H13NO/c1-10(2,3)8-6-4-5-7-9(8)11/h4-7H,1-3H3
InchiKey: VDAMZFHTCKFXBJ-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: C[N+](C)(C)c1ccccc1[O-]
Mol. weight [g/mol]: 151.21
CAS: 31061-58-2

Physical Properties

Property code	Value	Unit	Source
ie	6.80	eV	NIST Webbook
log10ws	1.68		Crippen Method
logp	0.957		Crippen Method
mcvol	129.760	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=C31061582&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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