

# 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](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/ci9903071>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/68-918-8/Benzenaminium-2-hydroxy-N-N-N-trimethyl-hydroxide-inner-salt.pdf>

Generated by Cheméo on 2024-04-23 18:12:43.761973912 +0000 UTC m=+16185212.682551228.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.