

# Betaine

<b>Other names:</b>	(carboxymethyl)trimethylammonium hydroxide
<b>Inchi:</b>	InChI=1S/C5H11NO2.H2O/c1-6(2,3)4-5(7)8;/h4H2,1-3H3;1H2
<b>InchiKey:</b>	NJZRLXNDBGZBREL-UHFFFAOYSA-N
<b>Formula:</b>	C5H13NO3
<b>SMILES:</b>	<chem>C[N+](C)(C)CC(=O)O.[OH-]</chem>
<b>Mol. weight [g/mol]:</b>	135.16
<b>CAS:</b>	590-47-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.72		Aqueous Solubility Prediction Method

## Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C590476&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

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