

# Trimethylene borate

<b>Other names:</b>	1,3,2-Dioxaborinane, 2,2'-[1,3-propanediylbis(oxy)]bis-2,2'-[propane-1,3-diylbis(oxy)]bis-1,3,2-dioxaborinane
<b>Inchi:</b>	InChI=1S/C9H18B2O6/c1-4-12-10(13-5-1)16-8-3-9-17-11-14-6-2-7-15-11/h1-9H2
<b>InchiKey:</b>	FZNHHPNJQSIEPT-UHFFFAOYSA-N
<b>Formula:</b>	C9H18B2O6
<b>SMILES:</b>	C1COB(OCCCOB2OCCCO2)OC1
<b>Mol. weight [g/mol]:</b>	243.86
<b>CAS:</b>	20905-35-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	3.60		Crippen Method
logp	0.253		Crippen Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20905355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20905355&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

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