

# Thiophene, 2,3-dibromo-

<b>Other names:</b>	2,3-Dibromothiophene
<b>Inchi:</b>	InChI=1S/C4H2Br2S/c5-3-1-2-7-4(3)6/h1-2H
<b>InchiKey:</b>	ATRJNSFQBYKFSM-UHFFFAOYSA-N
<b>Formula:</b>	C4H2Br2S
<b>SMILES:</b>	Brc1ccsc1Br
<b>Mol. weight [g/mol]:</b>	241.93
<b>CAS:</b>	3140-93-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.55		Crippen Method
logp	3.273		Crippen Method
mcvol	99.110	ml/mol	McGowan Method
rinpol	1227.00		NIST Webbook
rinpol	1227.00		NIST Webbook
tb	491.70	K	NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3140930&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3140930&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
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

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