

# Thiophene, 2-bromo-3-methyl-

<b>Other names:</b>	2-Bromo-3-methylthiophene
<b>Inchi:</b>	InChI=1S/C5H5BrS/c1-4-2-3-7-5(4)6/h2-3H,1H3
<b>InchiKey:</b>	YYJBWYBULYUKMR-UHFFFAOYSA-N
<b>Formula:</b>	C5H5BrS
<b>SMILES:</b>	Cc1ccsc1Br
<b>Mol. weight [g/mol]:</b>	177.06
<b>CAS:</b>	14282-76-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	2.819		Crippen Method
mcvol	95.700	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	300.20	K	0.30	NIST Webbook

## Sources

<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>
<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=C14282769&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14282769&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**tbrp:** Boiling point at reduced pressure

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