

2,5-Dibromo-3-methylthiophene

Other names:	Thiophene, 2,5-dibromo-3-methyl-
Inchi:	InChI=1S/C5H4Br2S/c1-3-2-4(6)8-5(3)7/h2H,1H3
InchiKey:	IHFZXROPBCBLLG-UHFFFAOYSA-N
Formula:	C5H4Br2S
SMILES:	Cc1cc(Br)sc1Br
Mol. weight [g/mol]:	255.96
CAS:	13191-36-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	3.582		Crippen Method
mcvol	113.200	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	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=C13191361&Units=SI

Legend

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/54-910-1/2-5-Dibromo-3-methylthiophene.pdf>

Generated by Cheméo on 2024-05-06 05:21:37.974420666 +0000 UTC m=+17262146.894997978.

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