

2,3,4-Tribromothiophene

Other names:	Thiophene, 2,3,4-tribromo-
Inchi:	InChI=1S/C4HBr3S/c5-2-1-8-4(7)3(2)6/h1H
InchiKey:	ZDXQFDMBZUQHOM-UHFFFAOYSA-N
Formula:	C4HBr3S
SMILES:	Brc1csc(Br)c1Br
Mol. weight [g/mol]:	320.83
CAS:	3141-25-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.72		Crippen Method
logp	4.036		Crippen Method
mcvol	116.610	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=C3141251&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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