

Benzo[b]thiophene, 3-bromo-

Other names:	3-Bromobenzo[b]thiophene
Inchi:	InChI=1S/C8H5BrS/c9-7-5-10-8-4-2-1-3-6(7)8/h1-5H
InchiKey:	SRWDQSRTOOMPMO-UHFFFAOYSA-N
Formula:	C8H5BrS
SMILES:	Brc1csc2ccccc12
Mol. weight [g/mol]:	213.09
CAS:	7342-82-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	3.664		Crippen Method
mcvol	118.510	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7342827&Units=SI
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

Legend

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

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<https://www.chemeo.com/cid/35-007-5/Benzo-b-thiophene-3-bromo.pdf>

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