

Benzo[c]thiophene

Inchi:	InChI=1S/C8H6S/c1-2-4-8-6-9-5-7(8)3-1/h1-6H
InchiKey:	LYTMVABTDYMBQK-UHFFFAOYSA-N
Formula:	C8H6S
SMILES:	c1ccc2csc2c1
Mol. weight [g/mol]:	134.20
CAS:	270-82-6

Physical Properties

Property code	Value	Unit	Source
ie	7.75	eV	NIST Webbook
log10ws	-3.03		Crippen Method
logp	2.901		Crippen Method
mcvol	101.010	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C270826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
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/34-976-1/Benzo-c-thiophene.pdf>

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