

[1]Benzothieno[3,2-b][1]benzothiophene

Other names: [1]Benzothiopheno[3,2-b][1]benzothiophene
Benzo[b]thieno[3,2-b]benzo[b]thiophene
Thianaphtheno[3,2-b]thianaphthene
Benzothieno[3,2-b]benzothiophene

Inchi: InChI=1S/C14H8S2/c1-3-7-11-9(5-1)13-14(15-11)10-6-2-4-8-12(10)16-13/h1-8H

InchiKey: NXCSDJOTXUWERI-UHFFFAOYSA-N

Formula: C14H8S2

SMILES: c1ccc2c(c1)sc1c3ccccc3sc21

Mol. weight [g/mol]: 240.34

CAS: 248-70-4

Physical Properties

Property code	Value	Unit	Source
ie	7.53	eV	NIST Webbook
log10ws	-6.40		Crippen Method
logp	5.269		Crippen Method
mcvol	167.280	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=C248704&Units=SI>

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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