

Benzo[4,5]phenaleno[9,1-bc]thiophene

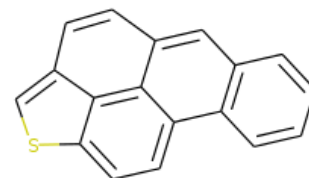
InChI: InChI=1S/C18H10S/c1-2-4-14-11(3-1)9-12-5-6-13-10-19-16-8-7-15(14)17(12)18(13)16/h1-10H

InChI Key: QWQMZHGXBGJJBB-UHFFFAOYSA-N

Formula: C18H10S

SMILES: c1sc2ccc3c4ccccc4cc4ccc1c2c43

Molecular Weight: 258.34



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	5.799		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H10S/c1-2-4-14-11\(3-1\)9-12-5-6-13-10-19-16-8-7-15\(14\)17\(12\)18\(13\)16/h1-10H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H10S/c1-2-4-14-11(3-1)9-12-5-6-13-10-19-16-8-7-15(14)17(12)18(13)16/h1-10H)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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