

Benzo[1,2-b:5,4-b']bis[1]benzothiophene

Other names: Benzo[1,2-b:5,4-b']bisthianaphthene.

InChI: InChI=1S/C18H10S2/c1-3-7-15-11(5-1)13-9-14-12-6-2-4-8-16(12)20-18(14)10-17(13)19-15/h1-10H

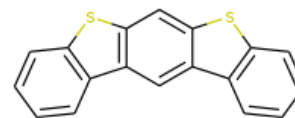
InChI Key: BRSOTWFOYHMQHJ-UHFFFAOYSA-N

Formula: C18H10S2

SMILES: c1ccc2c(c1)sc1cc3sc4ccccc4c3cc12

Molecular Weight: 290.40

CAS: 241-37-2



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	6.42		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H10S2/c1-3-7-15-11\(5-1\)13-9-14-12-6-2-4-8-16\(12\)20-18\(14\)10-17\(13\)19-15/h1-10H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H10S2/c1-3-7-15-11(5-1)13-9-14-12-6-2-4-8-16(12)20-18(14)10-17(13)19-15/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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