

Dinaphtho[1,2,-b:2',3'-d]thiophene

Other names: Dinaphtho[1,2-b;2',3-d]thiophene.

InChI: InChI=1S/C20H12S/c1-2-7-15-12-19-18(11-14(15)6-1)17-10-9-13-5-3-4-8-16(13)20(17)21-19/h1-12H

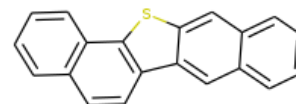
InChI Key: GHHYLNANHKNUED-UHFFFAOYSA-N

Formula: C₂₀H₁₂S

SMILES: c1ccc2c3sc4cc5ccccc5cc4c3ccc2c1

Molecular Weight: 284.37

CAS: 239-94-1



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	6.36		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H12S/c1-2-7-15-12-19-18\(11-14\(15\)6-1\)17-10-9-13-5-3-4-8-16\(13\)20\(17\)21-19/h1-12H](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H12S/c1-2-7-15-12-19-18(11-14(15)6-1)17-10-9-13-5-3-4-8-16(13)20(17)21-19/h1-12H)

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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