

# 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)2 |
| InchiKey:            | GHHYLNANHKNUED-UHFFFAOYSA-N                                                       |
| Formula:             | C20H12S                                                                           |
| SMILES:              | c1ccc2cc3c(cc2c1)sc1c2ccccc2ccc31                                                 |
| Mol. weight [g/mol]: | 284.37                                                                            |
| CAS:                 | 239-94-1                                                                          |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -8.45   |        | Crippen Method |
| logp          | 6.361   |        | Crippen Method |
| mcvol         | 211.710 | ml/mol | McGowan Method |
| rinpol        | 489.14  |        | NIST Webbook   |
| rinpol        | 489.14  |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C239941&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C239941&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| mcvol:   | McGowan's characteristic volume     |
| rinpol:  | Non-polar retention indices         |

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<https://www.chemeo.com/cid/77-609-1/Dinaphtho-1-2-b-2-3-d-thiophene.pdf>

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