

Perylo[1,12-bcd]thiophene

Inchi: InChI=1S/C20H10S/c1-3-11-7-9-15-19-17(11)13(5-1)14-6-2-4-12-8-10-16(21-15)20(19)1
InchiKey: BBANANIMTSEOOP-UHFFFAOYSA-N
Formula: C20H10S
SMILES: c1cc2ccc3sc4ccc5cccc6c(c1)c2c3c4c56
Mol. weight [g/mol]: 282.36
CAS: 31473-75-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -9.08 | | Crippen Method |
| logp | 6.390 | | Crippen Method |
| mcvol | 200.850 | ml/mol | McGowan Method |
| rinpol | 499.10 | | NIST Webbook |
| rinpol | 498.70 | | NIST Webbook |
| rinpol | 499.10 | | NIST Webbook |
| rinpol | 498.70 | | NIST Webbook |

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=C31473753&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/77-599-3/Perylo-1-12-bcd-thiophene.pdf>

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