

Anthra[2,3-b]benzo[d]thiophene

Inchi: InChI=1S/C20H12S/c1-2-6-14-10-16-12-20-18(11-15(16)9-13(14)5-1)17-7-3-4-8-19(17)2
InchiKey: SARKSIVGGPWEIF-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2cc3cc4c(cc3cc2c1)sc1cccc14
Mol. weight [g/mol]: 284.37

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	498.10		NIST Webbook
rinpol	497.60		NIST Webbook
rinpol	495.70		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R186279&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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/46-050-5/Anthra-2-3-b-benzo-d-thiophene.pdf>

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