

Benzo[7,8]anthro[2,1-b]thiophene, 5-methyl

Inchi: InChI=1S/C21H14S/c1-13-8-21-18(6-7-22-21)20-12-17-10-15-5-3-2-4-14(15)9-16(17)11-
InchiKey: RVCDUCKIZMLYJC-UHFFFAOYSA-N
Formula: C21H14S
SMILES: Cc1cc2sccc2c2cc3cc4ccccc4cc3cc12
Mol. weight [g/mol]: 298.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	6.669		Crippen Method
mcvol	225.800	ml/mol	McGowan Method
rinpole	511.30		NIST Webbook

Sources

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=R642581&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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