

Benzo[4,5]phenaleno[1,9]bc]thiophene

Inchi: InChI=1S/C18H10S/c1-2-4-14-11(3-1)9-12-6-8-16-18-13(10-19-16)5-7-15(14)17(12)18/h
InchiKey: NWJOURGNOOYFF-UHFFFAOYSA-N
Formula: C18H10S
SMILES: c1ccc2c(c1)cc1ccc3scc4ccc2c1c43
Mol. weight [g/mol]: 258.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.86		Crippen Method
logp	5.799		Crippen Method
mcvol	187.830	ml/mol	McGowan Method
rinpol	446.60		NIST Webbook
rinpol	446.30		NIST Webbook
rinpol	446.60		NIST Webbook
rinpol	456.20		NIST Webbook
rinpol	456.49		NIST Webbook
rinpol	455.09		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R21130&Units=SI>
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>

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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