

Chryseno-di[4,5-bcd:10,11-bcd]thiophene

Inchi: InChI=1S/C18H8S2/c1-3-9-7-13-18-16-10(4-2-6-12(16)20-13)8-14-17(18)15(9)11(5-1)19
InchiKey: HXWQWOBHTZUZPR-UHFFFAOYSA-N
Formula: C18H8S2
SMILES: c1cc2cc3sc4cccc5cc6sc(c1)c2c6c3c54
Mol. weight [g/mol]: 288.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.84		Crippen Method
logp	6.451		Crippen Method
mcvol	193.320	ml/mol	McGowan Method
rinpol	515.50		NIST Webbook
rinpol	521.80		NIST Webbook
rinpol	515.50		NIST Webbook
rinpol	521.80		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R186373&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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