

Chryseno[4,5-bcd]thiophene

Inchi: InChI=1S/C18H10S/c1-2-6-13-12(4-1)10-16-18-14(13)9-8-11-5-3-7-15(19-16)17(11)18/h
InchiKey: OKEYYZJTTUDDGO-UHFFFAOYSA-N
Formula: C18H10S
SMILES: c1ccc2c(c1)cc1sc3cccc4ccc2c1c43
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	450.36		NIST Webbook
rinpol	451.43		NIST Webbook
rinpol	450.62		NIST Webbook
rinpol	451.00		NIST Webbook
rinpol	442.20		NIST Webbook
rinpol	441.50		NIST Webbook
rinpol	441.90		NIST Webbook
rinpol	442.20		NIST Webbook
rinpol	451.00		NIST Webbook
rinpol	450.36		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R21439&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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