

Triphenyleno[4,5]thiophene

Inchi: InChI=1S/C18H10S/c1-2-6-12-11(5-1)13-7-3-9-15-17(13)18-14(12)8-4-10-16(18)19-15/h
InchiKey: GFFHWPBASMPTYKN-UHFFFAOYSA-N
Formula: C18H10S
SMILES: c1ccc2c(c1)c1cccc3sc4cccc2c4c31
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	445.10		NIST Webbook
rinpol	445.10		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=R643173&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/78-247-2/Triphenyleno-4-5-thiophene.pdf>

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