

Pyreno[4,5]thiophene

Inchi: InChI=1S/C18H10S/c1-3-11-7-8-12-4-2-6-15-17(12)16(11)13(5-1)14-9-10-19-18(14)15/h
InchiKey: KDHDCHNSCYZWIN-UHFFFAOYSA-N
Formula: C18H10S
SMILES: c1cc2ccc3cccc4c5sccc5c(c1)c2c34
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	443.68		NIST Webbook
rinpol	443.68		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R643153&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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<https://www.cheméo.com/cid/73-776-0/Pyreno-4-5-thiophene.pdf>

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