

Pyreno[4,5-b]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: KDHDCHNSCYZWJN-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	446.90		NIST Webbook
rinpol	446.51		NIST Webbook
rinpol	438.00		NIST Webbook
rinpol	438.50		NIST Webbook
rinpol	446.90		NIST Webbook
rinpol	438.00		NIST Webbook
rinpol	446.74		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R21756&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/68-819-8/Pyreno-4-5-b-thiophene.pdf>

Generated by Cheméo on 2024-04-18 20:13:33.982895603 +0000 UTC m=+15760462.903472914.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.