

Chryseno[4,5]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: OKEYYZJTUDDGO-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	447.08		NIST Webbook
rinpol	447.08		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R642769&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.chemeo.com/cid/77-089-9/Chryseno-4-5-thiophene.pdf>

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