

Phenaleno[1,9-bc]thiophene

Inchi: InChI=1S/C14H8S/c1-2-9-4-5-11-8-15-12-7-6-10(3-1)13(9)14(11)12/h1-8H
InchiKey: RIYPNUWTALNKLM-UHFFFAOYSA-N
Formula: C14H8S
SMILES: c1cc2ccc3csc4ccc(c1)c2c34
Mol. weight [g/mol]: 208.28
CAS: 79965-99-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.06		Crippen Method
logp	4.646		Crippen Method
mcvol	150.930	ml/mol	McGowan Method
rinpol	347.28		NIST Webbook
rinpol	354.83		NIST Webbook
rinpol	347.28		NIST Webbook
rinpol	354.83		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C79965994&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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