

Naphtho[1,2-c] or [2,3-c]thiophene

Inchi: InChI=1S/C12H8S/c1-2-4-11-9(3-1)5-6-10-7-13-8-12(10)11/h1-8H
InchiKey: YPEFMQGGABUYFX-UHFFFAOYSA-N
Formula: C12H8S
SMILES: c1ccc2c(c1)ccc1csc12
Mol. weight [g/mol]: 184.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	4.054		Crippen Method
mcvol	137.910	ml/mol	McGowan Method
rinpol	302.08		NIST Webbook
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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=R131427&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/51-989-8/Naphtho-1-2-c-or-2-3-c-thiophene.pdf>

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