Dinaphtho(1,2-b:2',1'-d)thiophene

Other names: 1,2,7,8-Dibenzo-9-thiafluorene
Inchi: InChI=1S/C20H12S/c1-3-7-15-13(5-1)9-11-17-18-12-10-14-6-2-4-8-16(14)20(18)21-19(1
InchiKey: RHACEINAFSEPBJ-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)ccc1c3ccc4ccccc4c3sc21
Mol. weight [g/mol]: 284.37
CAS: 239-72-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.45		Crippen Method
logp	6.361		Crippen Method
mcvol	211.710	ml/mol	McGowan Method
rinpol	482.60		NIST Webbook
rinpol	483.24		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C239725&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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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