

Triphenylene[2,1-b]thiophene

Inchi: InChI=1S/C20H12S/c1-2-7-15-13(5-1)14-6-3-4-8-16(14)20-17(15)9-10-19-18(20)11-12-2
InchiKey: SOSIJULCFHJNTI-UHFFFAOYSA-N
Formula: C20H12S
SMILES: c1ccc2c(c1)c1cccc1c1c3ccsc3ccc21
Mol. weight [g/mol]: 284.37
CAS: 80819-45-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.45		Crippen Method
logp	6.361		Crippen Method
mccvol	211.710	ml/mol	McGowan Method
rinpol	491.08		NIST Webbook
rinpol	492.80		NIST Webbook
rinpol	489.20		NIST Webbook
rinpol	489.00		NIST Webbook
rinpol	490.50		NIST Webbook
rinpol	491.08		NIST Webbook
rinpol	493.90		NIST Webbook
rinpol	490.50		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C80819450&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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