

Benzo[4,5]triphenyleno[1,12-bcd]thiophene

Inchi: InChI=1S/C20H10S/c1-3-11-7-8-12-9-10-16-20-18(12)17(11)13(4-1)14-5-2-6-15(21-16)1
InchiKey: WHZPICCZOUXVFW-UHFFFAOYSA-N
Formula: C20H10S
SMILES: c1cc2ccc3ccc4sc5cccc6c(c1)c2c3c4c56
Mol. weight [g/mol]: 282.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.08		Crippen Method
logp	6.390		Crippen Method
mcvol	200.850	ml/mol	McGowan Method
rinpol	499.80		NIST Webbook
rinpol	499.90		NIST Webbook
rinpol	497.10		NIST Webbook

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=R186313&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/64-635-6/Benzo-4-5-triphenyleno-1-12-bcd-thiophene.pdf>

Generated by Cheméo on 2024-04-23 11:36:34.674642717 +0000 UTC m=+16161443.595220032.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.