

Benzo[1,2]phenylene[3,4-bc]thiophene

Inchi: InChI=1S/C24H14S/c1-3-9-17-15(7-1)16-8-2-4-10-18(16)23-21-13-14-25-24(21)20-12-6-
InchiKey: GKZCUQLYQUDLOR-UHFFFAOYSA-N
Formula: C24H14S
SMILES: c1ccc2c(c1)c1ccccc1c1c3ccsc3c3ccccc3c21
Mol. weight [g/mol]: 334.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.25		Crippen Method
logp	7.514		Crippen Method
mcvol	248.610	ml/mol	McGowan Method

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=R642487&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/72-358-5/Benzo-1-2-phenylene-3-4-bc-thiophene.pdf>

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