

Benzo[1,2-b:5,4-b']bis[1]benzothiophene

Other names:	Benzo[1,2-b:5,4-b']bisthianaphthene
Inchi:	InChI=1S/C18H10S2/c1-3-7-15-11(5-1)13-9-14-12-6-2-4-8-16(12)20-18(14)10-17(13)19-
InchiKey:	BRSOTWFOYHMQHJ-UHFFFAOYSA-N
Formula:	C18H10S2
SMILES:	c1ccc2c(c1)sc1cc3sc4ccccc4c3cc12
Mol. weight [g/mol]:	290.40
CAS:	241-37-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.20		Crippen Method
logp	6.422		Crippen Method
mcvol	204.180	ml/mol	McGowan Method
rinpol	502.08		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C241372&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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