

Benzo[b]thiophene, 2-(2-naphthalenyl)-

Other names:	Benzo[b]thiophene, 2-(2-naphthyl)- 2-(2-Naphthyl)benzo[b]thiophene 2-(2-Naphthyl)-1-thiaindene 2-(2-Naphthyl)-1-benzothiophene 2-(2-Naphthalenyl)benzo[b]thiophene 2-(2'-naphthyl)-benzo[b]thiophene 2-(2-Naphthyl)benzothiophene
Inchi:	InChI=1S/C18H12S/c1-2-6-14-11-16(10-9-13(14)5-1)18-12-15-7-3-4-8-17(15)19-18/h1-11
InchiKey:	VXNMJAGOXHIGRF-UHFFFAOYSA-N
Formula:	C18H12S
SMILES:	<chem>c1ccc2cc(-c3cc4ccccc4s3)ccc2c1</chem>
Mol. weight [g/mol]:	260.35
CAS:	17164-77-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.44		Crippen Method
logp	5.721		Crippen Method
mccvol	198.690	ml/mol	McGowan Method
rinpol	430.65		NIST Webbook
rinpol	428.11		NIST Webbook
rinpol	425.50		NIST Webbook
rinpol	430.65		NIST Webbook

Sources

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=C17164771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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.cheméo.com/cid/34-402-7/Benzo-b-thiophene-2-2-naphthalenyl.pdf>

Generated by Cheméo on 2024-04-27 10:36:19.028612842 +0000 UTC m=+16503427.949190155.

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