

Benzo[b]naphtho[2,3-d]thiophene, 8-methyl-

Other names:	8-Methylnaphtho[2,3-b][1]benzothiophene 8-Methylbenzo[b]naphtho[2,3-d]thiophene Benzo[b]naphtho[2,3]thiophene, 8-methyl
Inchi:	InChI=1S/C17H12S/c1-11-6-7-12-9-15-14-4-2-3-5-16(14)18-17(15)10-13(12)8-11/h2-10H
InchiKey:	AHDCOIWBTWIVLJ-UHFFFAOYSA-N
Formula:	C17H12S
SMILES:	<chem>Cc1ccc2cc3c(cc2c1)sc1cccc13</chem>
Mol. weight [g/mol]:	248.34
CAS:	24964-07-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.516		Crippen Method
mccvol	188.900	ml/mol	McGowan Method
rinpol	412.41		NIST Webbook
rinpol	414.68		NIST Webbook
rinpol	413.75		NIST Webbook
rinpol	413.75		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24964076&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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