

Benzo[b]thiophene, 4-nonyl

Other names:	4-Nonylbenzo[b]thiophene
Inchi:	InChI=1S/C17H24S/c1-2-3-4-5-6-7-8-10-15-11-9-12-17-16(15)13-14-18-17/h9,11-14H,2-
InchiKey:	BRFXDRPYWVUZKV-UHFFFAOYSA-N
Formula:	C17H24S
SMILES:	CCCCCCCCCc1cccc2sccc12
Mol. weight [g/mol]:	260.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.77		Crippen Method
logp	6.194		Crippen Method
mcvol	227.820	ml/mol	McGowan Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		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=R41641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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<https://www.chemeo.com/cid/58-955-8/Benzo-b-thiophene-4-nonyl.pdf>

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