

2,5-Bis(5-tert-butyl-2-benzoxazolyl)thiophene

Other names:	2,5-Bis(5-t-butylbenzoxazol-2-yl)thiophene 2,5-Bis(5-tert-butylbenzoxazol-2-yl)thiophene Benzoxazole, 2,2'-(2,5-thiophenediyl)bis[5-(1,1-dimethylethyl)-2,5-Bis-2(5-tert-butylbenzoxazolyl)thiophene 2,5-Bis(5-tert-butylbenzoxazolyl)-2-thiophene Benzoxazole, 2,2'-(2,5-thiophenediyl)bis(5-tert-butyl-BBOT 2,2'-(2,5-Thiophenediyl)bis(5-tert-butylbenzoxazole) 2,5-Bis(5'-tert-butyl-2-benzoxazolyl)thiophene BBOT 150 NSC 158163 Uvitex OB 2,5-thiophenediylbis(5-tert-butyl-1,3-benzoxazole)
Inchi:	InChI=1S/C26H26N2O2S/c1-25(2,3)15-7-9-19-17(13-15)27-23(29-19)21-11-12-22(31-21
InchiKey:	AIXZBGVLRQSS-UHFFFAOYSA-N
Formula:	C26H26N2O2S
SMILES:	CC(C)(C)c1ccc2oc(-c3ccc(-c4nc5cc(C(C)(C)C)ccc5o4)s3)nc2c1
Mol. weight [g/mol]:	430.56
CAS:	7128-64-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-19.67		Crippen Method
logp	7.959		Crippen Method
mccvol	327.950	ml/mol	McGowan Method
rinpol	3750.00		NIST Webbook
rinpol	3750.00		NIST Webbook
rinpol	3750.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7128645&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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