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

Other names: 2,2':5',2''-Diepoxy-p-terphenyl
1,1':4',1''-Terphenyl, 2,2':5',2''-diepoxy-
1,1':4',1''-Terphenyl, 2,2':5',2''-dioxido-
2,2':5',2''-Diepoxy-1,1':4',1''-terphenyl
2,2':5,2''-Dioxido-1,1':4',1''-terphenyl
Dibenzo[d,d']benzo[1,2-b; 4,5-b']difuran

Inchi: InChI=1S/C18H10O2/c1-3-7-15-11(5-1)13-9-18-14(10-17(13)19-15)12-6-2-4-8-16(12)20-

InchiKey: RVAFAAJAGUSYCC-UHFFFAOYSA-N

Formula: C18H10O2

SMILES: c1ccc2c(c1)oc1cc3c(cc12)oc1ccccc13

Mol. weight [g/mol]: 258.27

CAS: 208-37-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.16		Crippen Method
logp	5.485		Crippen Method
mcvol	183.220	ml/mol	McGowan Method
rinpol	410.06		NIST Webbook
rinpol	410.06		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C208377&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