

Triphenyleno[1,12-bcd; 4,5-b'c'd']difuran

Inchi:	InChI=1S/C18H8O2/c1-3-9-10-4-2-6-12-16(10)18-14(20-12)8-7-13-17(18)15(9)11(5-1)19
InchiKey:	WTXVFBVAQYRKKT-UHFFFAOYSA-N
Formula:	C18H8O2
SMILES:	c1cc2oc3ccc4oc5cccc6c(c1)c2c3c4c56
Mol. weight [g/mol]:	256.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.79		Crippen Method
logp	5.514		Crippen Method
mcvol	172.360	ml/mol	McGowan Method
rinpola	401.82		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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