

Dinaphtho[2,1-b:1',2'-d]furan

Inchi:	InChI=1S/C20H12O/c1-3-7-15-13(5-1)9-11-17-19(15)20-16-8-4-2-6-14(16)10-12-18(20)2
InchiKey:	QIMOZEUDRUTIBS-UHFFFAOYSA-N
Formula:	C20H12O
SMILES:	c1ccc2c(c1)ccc1oc3ccc4ccccc4c3c12
Mol. weight [g/mol]:	268.31
CAS:	194-63-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.42		Crippen Method
logp	5.892		Crippen Method
mcvol	201.230	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C194638&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

Latest version available from:

<https://www.chemeo.com/cid/40-492-1/Dinaphtho-2-1-b-1-2-d-furan.pdf>

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