

Dinaphtho[2,1-b;2',3'-d]furan

Inchi: InChI=1S/C20H12O/c1-2-7-15-12-19-17(11-14(15)6-1)20-16-8-4-3-5-13(16)9-10-18(20)2
InchiKey: KIOUONCGDXYZNB-UHFFFAOYSA-N
Formula: C20H12O
SMILES: c1ccc2cc3c(cc2c1)oc1ccc2ccccc2c13
Mol. weight [g/mol]: 268.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.42		Crippen Method
logp	5.892		Crippen Method
mcvol	201.230	ml/mol	McGowan Method
rinpol	447.40		NIST Webbook
rinpol	447.40		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R559063&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices

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