

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

Other names: Dinaphtho[1,2-b;1',2'-d]furan
Inchi: InChI=1S/C20H12O/c1-3-7-15-13(5-1)10-12-18-19(15)17-11-9-14-6-2-4-8-16(14)20(17)2
InchiKey: MNXYJVWXMUBENA-UHFFFAOYSA-N
Formula: C20H12O
SMILES: c1ccc2c(c1)ccc1c2oc2ccc3ccccc3c21
Mol. weight [g/mol]: 268.31
CAS: 207-93-2

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	450.20		NIST Webbook
rinpol	440.10		NIST Webbook
rinpol	440.10		NIST Webbook
rinpol	450.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C207932&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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<https://www.chemeo.com/cid/72-749-1/Dinaphtho-1-2-b-1-2-d-furan.pdf>

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