3-Methyldibenzofuran

Inchi: InChI=1S/C13H10O/c1-9-6-7-11-10-4-2-3-5-12(10)14-13(11)8-9/h2-8H,1H3
InchiKey: JBFNQSFELCVNBC-UHFFFAOYSA-N
Formula: C13H10O
SMILES: Cc1ccc2c(c1)oc1ccccc12
Mol. weight [g/mol]: 182.22
CAS: 7320-52-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.29		Crippen Method
logp	3.894		Crippen Method
mcvol	141.520	ml/mol	McGowan Method
rinpol	1612.00		NIST Webbook
rinpol	273.36		NIST Webbook
rinpol	273.65		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7320527&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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