

1-Methyldibenzofuran

Inchi: InChI=1S/C13H10O/c1-9-5-4-8-12-13(9)10-6-2-3-7-11(10)14-12/h2-8H,1H3
InchiKey: GGXKQILBNJUKSH-UHFFFAOYSA-N
Formula: C13H10O
SMILES: Cc1cccc2oc3ccccc3c12
Mol. weight [g/mol]: 182.22
CAS: 7320-50-5

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	274.89		NIST Webbook
rinpol	275.56		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7320505&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/13-359-9/1-Methyldibenzofuran.pdf>

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