Dibenzofuran, 4-methyl-

Other names: 4-Methyldibenzofuran
Inchi: InChI=1S/C13H10O/c1-9-5-4-7-11-10-6-2-3-8-12(10)14-13(9)11/h2-8H,1H3
InchiKey: XLTFRTTTZWMJJQ-UHFFFAOYSA-N
Formula: C13H10O
SMILES: Cc1cccc2c1oc1ccccc12
Mol. weight [g/mol]: 182.22
CAS: 7320-53-8

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	1638.00		NIST Webbook
rinpol	279.10		NIST Webbook
rinpol	271.38		NIST Webbook
rinpol	271.30		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7320538&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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