5-methyl-1(3H)-isobenzofuran

Inchi: InChI=1S/C9H8O/c1-7-2-3-8-5-10-6-9(8)4-7/h2-6H,1H3
InchiKey: BJCGCTDHYXCSTL-UHFFFAOYSA-N
Formula: C9H8O
SMILES: Cc1ccc2cocc2c1
Mol. weight [g/mol]: 132.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.49		Crippen Method
logp	2.741		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
rinpol	1159.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R216276&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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