3-Phenyl-benzofuran

Other names: 3-Phenylbenzo[b]furan
Inchi: InChI=1S/C14H10O/c1-2-6-11(7-3-1)13-10-15-14-9-5-4-8-12(13)14/h1-10H
InchiKey: SSYBGLWXGRWEFE-UHFFFAOYSA-N
Formula: C14H10O
SMILES: c1ccc(-c2coc3ccccc23)cc1
Mol. weight [g/mol]: 194.23
CAS: 29909-72-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.61		Crippen Method
logp	4.100		Crippen Method
mcvol	151.310	ml/mol	McGowan Method
rinpol	296.10		NIST Webbook
rinpol	296.10		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29909726&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

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