

1-Phenyldibenzofuran

Inchi: InChI=1S/C18H12O/c1-2-7-13(8-3-1)14-10-6-12-17-18(14)15-9-4-5-11-16(15)19-17/h1-1
InchiKey: PABWCQBWXPHCBX-UHFFFAOYSA-N
Formula: C18H12O
SMILES: c1ccc(-c2cccc3oc4ccccc4c23)cc1
Mol. weight [g/mol]: 244.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.42		Crippen Method
logp	5.253		Crippen Method
mcvol	188.210	ml/mol	McGowan Method
rinpola	359.53		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U314394&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
rinpola: Non-polar retention indices

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