

2-Diphenyl-carbinol-benzofuran

Inchi:	InChI=1S/C21H16O2/c22-21(20-14-18-8-4-5-9-19(18)23-20)17-12-10-16(11-13-17)15-6-
InchiKey:	ARCUPWRDHYITA-UHFFFAOYSA-N
Formula:	C21H16O2
SMILES:	OC(c1ccc(-c2ccccc2)cc1)c1cc2ccccc2o1
Mol. weight [g/mol]:	300.35
CAS:	82158-27-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.44		Crippen Method
logp	5.181		Crippen Method
mcvol	232.050	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82158278&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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