6-isopropyl-4-methyl-7,8-dihydro-6H-naphtho[1,8-bc]furan (acorafuran)

Inchi: InChI=1S/C15H18O/c1-9(2)12-4-5-14-15-11(8-16-14)6-10(3)7-13(12)15/h6-9,12H,4-5H2

InchiKey: ODMJVNAWLXWZED-UHFFFAOYSA-N

Formula: C15H18O

SMILES: Cc1cc2c3c(occ3c1)CCC2C(C)C

Mol. weight [g/mol]: 214.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.54		Crippen Method
logp	4.427		Crippen Method
mcvol	178.300	ml/mol	McGowan Method
rinpol	1735.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R514684&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices