Verboccidentafuran

Inchi: InChI=1S/C15H20O/c1-9-4-5-12-10(2)7-14-15(13(12)6-9)11(3)8-16-14/h6,8,10,12-13H,4
InchiKey: YONZCIKAMCMODD-QFWMXSHPSA-N
Formula: C15H20O
SMILES: CC1=CC2c3c(C)coc3CC(C)C2CC1
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	4.220		Crippen Method
mcvol	182.600	ml/mol	McGowan Method
rinpol	1662.00		NIST Webbook
rinpol	1665.00		NIST Webbook
ripol	2144.00		NIST Webbook
ripol	2130.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R320979&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices