Isofuranodienone

Inchi: InChI=1S/C15H18O2/c1-10-5-4-6-11(2)8-14-15(13(16)7-10)12(3)9-17-14/h6-7,9H,4-5,8H
InchiKey: XVOHELPNOXGRBQ-IKVLVDHLSA-N
Formula: C15H18O2
SMILES: CC1=CC(=O)c2c(C)coc2CC(C)=CCC1
Mol. weight [g/mol]: 230.30
CAS: 24268-42-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.26		Crippen Method
logp	4.000		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
rinpol	1814.10		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=C24268426&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.