

Furanodienone

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-NXAIOARDSA-N
Formula:	C15H18O2
SMILES:	CC1=CC(=O)c2c(C)coc2CC(C)=CCC1
Mol. weight [g/mol]:	230.30
CAS:	24268-41-5

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	1792.90		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1752.00		NIST Webbook
ripol	2240.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24268415&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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<https://www.chemeo.com/cid/85-122-2/Furanodienone.pdf>

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