

4(5H)-Benzofuranone, 6,7-dihydro-3,6-dimethyl-, (R)-

Other names:	Evodone (R)-3,6-Dimethyl-6,7-dihydrobenzofuran-4(5H)-one
Inchi:	InChI=1S/C10H12O2/c1-6-3-8(11)10-7(2)5-12-9(10)4-6/h5-6H,3-4H2,1-2H3/t6-/m1/s1
InchiKey:	SMUXTLISYBPIAU-ZCFIWIBFSA-N
Formula:	C10H12O2
SMILES:	<chem>Cc1coc2c1C(=O)CC(C)C2</chem>
Mol. weight [g/mol]:	164.20
CAS:	529-63-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.22		Crippen Method
logp	2.353		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
rinpol	1347.30		NIST Webbook
rinpol	1347.30		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2020.00		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=C529635&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

ripol: Polar retention indices

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