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: Cc1coc2c1C(=O)CC(C)C2
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