3,4-Dimethyl-6-tert-butylcoumarin

Inchi: InChI=1S/C15H18O2/c1-9-10(2)14(16)17-13-7-6-11(8-12(9)13)15(3,4)5/h6-8H,1-5H3
InchiKey: RZUCTRVCMQEVFR-UHFFFAOYSA-N
Formula: C15H18O2
SMILES: Cc1c(C)c2cc(C(C)(C)C)ccc2oc1=O
Mol. weight [g/mol]: 230.30
CAS: 116373-39-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.70		Crippen Method
logp	3.707		Crippen Method
mcvol	190.730	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373398&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