

# 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

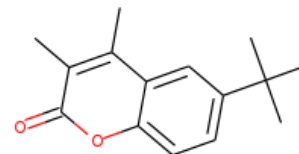
**InChI Key:** RZUCTRVCMQEVFR-UHFFFAOYSA-N

**Formula:** C<sub>15</sub>H<sub>18</sub>O<sub>2</sub>

**SMILES:** Cc1c(C)c(=O)oc2ccc(C(C)(C)C)cc12

**Molecular Weight:** 230.30

**CAS:** 116373-39-8



## Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	3.707		Crippen Method

## Sources

**NIST Webbook:** [http://webbook.nist.gov/cgi/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](http://webbook.nist.gov/cgi/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)

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

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