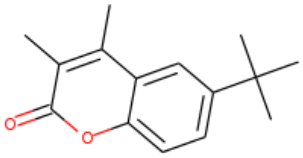
3,4-Dimethyl-6-tert-butylcoumarin

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: C15H18O2
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$_{oct/wat}$	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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .