

6-tert-Butyl-4-methylcoumarin

Other names:	6-t-Butyl-4-methylcoumarin
Inchi:	InChI=1S/C14H16O2/c1-9-7-13(15)16-12-6-5-10(8-11(9)12)14(2,3)4/h5-8H,1-4H3
InchiKey:	BVQZHRREUVIRFZ-UHFFFAOYSA-N
Formula:	C14H16O2
SMILES:	<chem>Cc1cc(=O)oc2ccc(C(C)(C)C)cc12</chem>
Mol. weight [g/mol]:	216.28
CAS:	17874-32-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.22		Crippen Method
logp	3.399		Crippen Method
mcvol	176.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17874327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/46-550-0/6-tert-Butyl-4-methylcoumarin.pdf>

Generated by Cheméo on 2024-04-26 20:36:32.659568722 +0000 UTC m=+16453041.580146037.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.