6-t-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: Cc1cc(=O)oc2ccc(C(C)(C)C)cc12
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
hvap	91.51	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-4.61		Cheméo Relay (1.0)
logp	3.399		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
tf	391.37	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17874327&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point