

7-Methoxy-8-(3-methyl-2-oxobutyl)-2H-chromen-2

Inchi: InChI=1S/C15H16O4/c1-9(2)12(16)8-11-13(18-3)6-4-10-5-7-14(17)19-15(10)11/h4-7,9H,
InchiKey: OMOYQLRHKFGVGN-UHFFFAOYSA-N
Formula: C15H16O4
SMILES: COc1ccc2ccc(=O)oc2c1CC(=O)C(C)C
Mol. weight [g/mol]: 260.29
CAS: 1088-17-1

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.65 | | Crippen Method |
| logp | 2.569 | | Crippen Method |
| mcvol | 198.170 | ml/mol | McGowan Method |
| rinpol | 2252.10 | | NIST Webbook |
| rinpol | 2248.10 | | NIST Webbook |
| rinpol | 2243.00 | | NIST Webbook |
| rinpol | 2243.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1088171&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices

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