

# DIMETHYLCHRYSIN

|                      |                                                                                                     |
|----------------------|-----------------------------------------------------------------------------------------------------|
| Other names:         | Flavone, 5,7-dimethoxy-<br>Chrysin - dimethyl ether<br>Dimethylchrysin<br>5,7-Dimethoxyflavone, TMS |
| Inchi:               | InChI=1S/C17H14O4/c1-19-12-8-15(20-2)17-13(18)10-14(21-16(17)9-12)11-6-4-3-5-7-11                   |
| InchiKey:            | JRFZSUMZAUHNSL-UHFFFAOYSA-N                                                                         |
| Formula:             | C17H14O4                                                                                            |
| SMILES:              | COc1cc(OC)c2c(=O)cc(-c3ccccc3)oc2c1                                                                 |
| Mol. weight [g/mol]: | 282.29                                                                                              |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| logp          | 3.477   |        | Crippen Method     |
| mcvol         | 206.890 | ml/mol | McGowan Method     |
| rinpol        | 2588.00 |        | NIST Webbook       |
| rinpol        | 2588.00 |        | NIST Webbook       |
| tf            | 419.02  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                               |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                     |
| Crippen Method:           | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                             |
| Cheméo Relay (1.0):       |                                                                                                                                               |
| Cheméo Relay (1.0, beta): |                                                                                                                                               |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21392574&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21392574&amp;Units=SI</a> |

## Legend

|        |                                     |
|--------|-------------------------------------|
| logp:  | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume     |

**rinpol:** Non-polar retention indices  
**tf:** Normal melting (fusion) point

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