

# 2H-1-BENZOPYRAN-2-ONE, 8-METHOXY-

|                      |                                                               |
|----------------------|---------------------------------------------------------------|
| Other names:         | Coumarin, 8-methoxy-                                          |
| Inchi:               | InChI=1S/C10H8O3/c1-12-8-4-2-3-7-5-6-9(11)13-10(7)8/h2-6H,1H3 |
| InchiKey:            | ODRDTKMYQDXVGG-UHFFFAOYSA-N                                   |
| Formula:             | C10H8O3                                                       |
| SMILES:              | COc1cccc2ccc(=O)oc12                                          |
| Mol. weight [g/mol]: | 176.17                                                        |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | -291.55 | kJ/mol | Cheméo Relay (1.0) |
| ie            | 8.36    | eV     | Cheméo Relay (1.0) |
| log10ws       | -2.37   |        | Cheméo Relay (1.0) |
| logp          | 1.802   |        | Crippen Method     |
| mcvol         | 126.150 | ml/mol | McGowan Method     |
| tb            | 605.86  | K      | Cheméo Relay (1.0) |
| tf            | 362.48  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                             |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                   |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=C2445810&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2445810&amp;Units=SI</a> |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|          |                                              |
|----------|----------------------------------------------|
| hf:      | Enthalpy of formation at standard conditions |
| ie:      | Ionization energy                            |
| log10ws: | Log10 of Water solubility in mol/l           |

|               |                                     |
|---------------|-------------------------------------|
| <b>logp:</b>  | Octanol/Water partition coefficient |
| <b>mcvol:</b> | McGowan's characteristic volume     |
| <b>tb:</b>    | Normal Boiling Point Temperature    |
| <b>tf:</b>    | Normal melting (fusion) point       |

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