

2H-Pyran-5-carboxylic acid, 2-oxo-, methyl ester

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| Other names: | 5-(Carbomethoxy)-2-pyrone Coumalic acid methyl ester Glutaconic acid, 4-(hydroxymethylene)-, «delta»-lactone, methyl ester Methyl coumalate Methyl 2-oxo-2H-pyran-5-carboxylate Methyl 2-pyrone-5-carboxylate |
| Inchi: | InChI=1S/C7H6O4/c1-10-7(9)5-2-3-6(8)11-4-5/h2-4H,1H3 |
| InchiKey: | HHWWWZQYHPFCBY-UHFFFAOYSA-N |
| Formula: | C7H6O4 |
| SMILES: | <chem>COC(=O)c1ccc(=O)oc1</chem> |
| Mol. weight [g/mol]: | 154.12 |
| CAS: | 6018-41-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.87 | | Crippen Method |
| logp | 0.426 | | Crippen Method |
| mcvol | 104.910 | ml/mol | McGowan Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 452.20 | K | 8.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6018413&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 |
| tbrp: | Boiling point at reduced pressure |

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