# 2H-1-Benzopyran-2-one, 7-methyl-

**Other names:** 7-Methylcoumarin
Coumarin, 7-methyl-
7-Methyl-2H-1-benzopyran-2-one
**Inchi:** InChI=1S/C10H8O2/c1-7-2-3-8-4-5-10(11)12-9(8)6-7/h2-6H,1H3
**InchiKey:** DLHXRDUXNVEIEY-UHFFFAOYSA-N
**Formula:** C10H8O2
**SMILES:** Cc1ccc2ccc(=O)oc2c1
**Mol. weight [g/mol]:** 160.17
**CAS:** 2445-83-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.91 | | Crippen Method |
| logp | 2.101 | | Crippen Method |
| mcvol | 120.280 | ml/mol | McGowan Method |
| rinpol | 1545.00 | | NIST Webbook |
| rinpol | 1562.00 | | NIST Webbook |
| rinpol | 1553.00 | | NIST Webbook |
| rinpol | 1574.00 | | NIST Webbook |
| rinpol | 1586.00 | | NIST Webbook |
| rinpol | 1553.00 | | NIST Webbook |
| ripol | 2620.00 | | NIST Webbook |
| ripol | 2620.00 | | NIST Webbook |

## Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 444.70 | K | 1.50 | NIST Webbook |

## Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2445832&Units=SI |

# Legend

| | |
|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tbrp:** | Boiling point at reduced pressure |