# 2H-1-Benzopyran-2-one, 7-amino-4-methyl-

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|---|---|
| **Other names:** | 7-Amino-4-methylcoumarin |
| | C 120 |
| | Coumarin 120 |
| | Coumarin 440 |
| | Coumarin, 7-Amino-4-methyl- |
| | 4-Methyl-7-aminocoumarin |
| **Inchi:** | InChI=1S/C10H9NO2/c1-6-4-10(12)13-9-5-7(11)2-3-8(6)9/h2-5H,11H2,1H3 |
| **InchiKey:** | GLNDAGDHSLMOKX-UHFFFAOYSA-N |
| **Formula:** | C10H9NO2 |
| **SMILES:** | Cc1cc(=O)oc2cc(N)ccc12 |
| **Mol. weight [g/mol]:** | 175.18 |
| **CAS:** | 26093-31-2 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 8.05 | eV | NIST Webbook |
| log10ws | -6.54 | | Crippen Method |
| logp | 1.684 | | Crippen Method |
| mcvol | 130.260 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| hfust | 32.09 | kJ/mol | 499.90 | NIST Webbook |
| hfust | 32.09 | kJ/mol | 499.90 | NIST Webbook |
| sfust | 64.82 | J/mol×K | 499.90 | NIST Webbook |

## Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C26093312&Units=SI |

# Legend

| | |
|---|---|
| **hfust:** | Enthalpy of fusion at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **sfust:** | Entropy of fusion at a given temperature |