# iso-Propyl n-methyl anthranilate

**Inchi:** InChI=1S/C11H15NO2/c1-8(2)14-11(13)9-6-4-5-7-10(9)12-3/h4-8,12H,1-3H3
**InchiKey:** OBKVPPPSOAFJDS-UHFFFAOYSA-N
**Formula:** C11H15NO2
**SMILES:** CNc1ccccc1C(=O)OC(C)C
**Mol. weight [g/mol]:** 193.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -332.75 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 22.26 | kJ/mol | Joback Method |
| ie | 7.73 | eV | Cheméo Relay (1.0) |
| log10ws | -3.13 | | Cheméo Relay (1.0) |
| logp | 2.293 | | Crippen Method |
| mcvol | 159.510 | ml/mol | McGowan Method |
| pc | 2796.51 | kPa | Joback Method |
| rinpol | 1491.00 | | NIST Webbook |
| rinpol | 1491.00 | | NIST Webbook |
| ripol | 2058.00 | | NIST Webbook |
| ripol | 2058.00 | | NIST Webbook |
| tb | 531.14 | K | Cheméo Relay (1.0) |
| tf | 302.19 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 396.17 | J/mol×K | 608.76 | Joback Method |
| cpg | 410.54 | J/mol×K | 644.51 | Joback Method |
| cpg | 424.06 | J/mol×K | 680.25 | Joback Method |
| cpg | 436.76 | J/mol×K | 716.00 | Joback Method |
| cpg | 448.64 | J/mol×K | 751.75 | Joback Method |
| cpg | 459.72 | J/mol×K | 787.50 | Joback Method |
| cpg | 470.03 | J/mol×K | 823.24 | Joback Method |

# Sources

| | |
|---|---|
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C99985645&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |