# 2'-Methylbutyrophenone

**Inchi:** InChI=1S/C11H14O/c1-3-6-11(12)10-8-5-4-7-9(10)2/h4-5,7-8H,3,6H2,1-2H3
**InchiKey:** ALQIJXZCLUTTIY-UHFFFAOYSA-N
**Formula:** C11H14O
**SMILES:** CCCC(=O)c1ccccc1C
**Mol. weight [g/mol]:** 162.23
**CAS:** 35028-06-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 15.60 | kJ/mol | Joback Method |
| hf | -157.89 | kJ/mol | Joback Method |
| hfus | 19.50 | kJ/mol | Joback Method |
| hvap | 49.76 | kJ/mol | Joback Method |
| log10ws | -3.44 | | Crippen Method |
| logp | 2.978 | | Crippen Method |
| mcvol | 143.660 | ml/mol | McGowan Method |
| pc | 2784.72 | kPa | Joback Method |
| rinpol | 1283.00 | | NIST Webbook |
| rinpol | 1283.00 | | NIST Webbook |
| tb | 536.61 | K | Joback Method |
| tc | 749.19 | K | Joback Method |
| tf | 302.60 | K | Joback Method |
| vc | 0.549 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 321.61 | J/mol×K | 536.61 | Joback Method |
| cpg | 336.08 | J/mol×K | 572.04 | Joback Method |
| cpg | 349.73 | J/mol×K | 607.47 | Joback Method |
| cpg | 362.58 | J/mol×K | 642.90 | Joback Method |
| cpg | 374.66 | J/mol×K | 678.33 | Joback Method |
| cpg | 386.00 | J/mol×K | 713.76 | Joback Method |
| cpg | 396.64 | J/mol×K | 749.19 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0022892 | Pa×s | 302.60 | Joback Method |
| dvisc | 0.0012638 | Pa×s | 341.60 | Joback Method |
| dvisc | 0.0007880 | Pa×s | 380.60 | Joback Method |
| dvisc | 0.0005365 | Pa×s | 419.60 | Joback Method |
| dvisc | 0.0003899 | Pa×s | 458.61 | Joback Method |
| dvisc | 0.0002979 | Pa×s | 497.61 | Joback Method |
| dvisc | 0.0002367 | Pa×s | 536.61 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C35028069&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |