# 2',6'-dimethylacetophenone

**Other names:** 2,6-(CH3)2C6H3-COCH3
**Inchi:** InChI=1S/C10H12O/c1-7-5-4-6-8(2)10(7)9(3)11/h4-6H,1-3H3
**InchiKey:** DDXBCZCBZGPSHD-UHFFFAOYSA-N
**Formula:** C10H12O
**SMILES:** CC(=O)c1c(C)cccc1C
**Mol. weight [g/mol]:** 148.20
**CAS:** 2142-76-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 857.00 | kJ/mol | NIST Webbook |
| basg | 825.20 | kJ/mol | NIST Webbook |
| gf | -2.45 | kJ/mol | Joback Method |
| hf | -148.72 | kJ/mol | Joback Method |
| hfus | 16.52 | kJ/mol | Joback Method |
| hvap | 48.20 | kJ/mol | Joback Method |
| log10ws | -3.08 | | Crippen Method |
| logp | 2.506 | | Crippen Method |
| mcvol | 129.570 | ml/mol | McGowan Method |
| pc | 3038.96 | kPa | Joback Method |
| tb | 518.71 | K | Joback Method |
| tc | 735.99 | K | Joback Method |
| tf | 293.92 ± 0.25 | K | NIST Webbook |
| vc | 0.493 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 276.59 | J/mol×K | 518.71 | Joback Method |
| cpg | 335.57 | J/mol×K | 699.77 | Joback Method |
| cpg | 325.13 | J/mol×K | 663.56 | Joback Method |
| cpg | 314.04 | J/mol×K | 627.35 | Joback Method |
| cpg | 302.26 | J/mol×K | 591.14 | Joback Method |
| cpg | 289.78 | J/mol×K | 554.92 | Joback Method |

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|---|---|---|---|---|
| cpg | 345.38 | J/mol×K | 735.99 | Joback Method |
| dvisc | 0.0002423 | Pa×s | 518.71 | Joback Method |
| dvisc | 0.0002973 | Pa×s | 482.90 | Joback Method |
| dvisc | 0.0003768 | Pa×s | 447.09 | Joback Method |
| dvisc | 0.0004977 | Pa×s | 411.28 | Joback Method |
| dvisc | 0.0006932 | Pa×s | 375.47 | Joback Method |
| dvisc | 0.0010355 | Pa×s | 339.66 | Joback Method |
| dvisc | 0.0017002 | Pa×s | 303.85 | 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=C2142769&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

**affp:** Proton affinity
**basg:** Gas basicity
**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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume