# 1,3-dimethyl-isochroman, 1e', 3e

**Inchi:** InChI=1S/C11H14O/c1-8-7-10-5-3-4-6-11(10)9(2)12-8/h3-6,8-9H,7H2,1-2H3/t8-,9+/m1/s
**InchiKey:** AIODYCJUHTYCEB-BDAKNGLRSA-N
**Formula:** C11H14O
**SMILES:** CC1Cc2ccccc2C(C)O1
**Mol. weight [g/mol]:** 162.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 99.34 | kJ/mol | Joback Method |
| hf | -131.01 | kJ/mol | Joback Method |
| hfus | 22.98 | kJ/mol | Joback Method |
| hvap | 47.30 | kJ/mol | Joback Method |
| log10ws | -3.05 | | Crippen Method |
| logp | 2.709 | | Crippen Method |
| mcvol | 137.100 | ml/mol | McGowan Method |
| pc | 2937.70 | kPa | Joback Method |
| rinpol | 1236.40 | | NIST Webbook |
| ripol | 1689.80 | | NIST Webbook |
| tb | 516.03 | K | Joback Method |
| tc | 742.26 | K | Joback Method |
| tf | 289.42 | K | Joback Method |
| vc | 0.512 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 318.39 | J/mol×K | 516.03 | Joback Method |
| cpg | 335.94 | J/mol×K | 553.74 | Joback Method |
| cpg | 352.37 | J/mol×K | 591.44 | Joback Method |
| cpg | 367.75 | J/mol×K | 629.15 | Joback Method |
| cpg | 382.12 | J/mol×K | 666.85 | Joback Method |
| cpg | 395.53 | J/mol×K | 704.56 | Joback Method |
| cpg | 408.03 | J/mol×K | 742.26 | Joback Method |
| dvisc | 0.0018157 | Pa×s | 289.42 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0012161 | Pa×s | 327.19 | Joback Method |
| dvisc | 0.0008849 | Pa×s | 364.96 | Joback Method |
| dvisc | 0.0006835 | Pa×s | 402.73 | Joback Method |
| dvisc | 0.0005518 | Pa×s | 440.49 | Joback Method |
| dvisc | 0.0004608 | Pa×s | 478.26 | Joback Method |
| dvisc | 0.0003951 | Pa×s | 516.03 | Joback Method |

# Sources

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|---|---|
| **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=R256690&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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