# Tricyclo[4.3.1.1(2,5)]undecane, 10-methoxy-, stereoisomer

**Inchi:** InChI=1S/C12H20O/c1-13-12-10-3-2-4-11(12)9-6-5-8(10)7-9/h8-12H,2-7H2,1H3
**InchiKey:** FZLYZEQLJWOGIF-UHFFFAOYSA-N
**Formula:** C12H20O
**SMILES:** COC1C2CCCC1C1CCC2C1
**Mol. weight [g/mol]:** 180.29
**CAS:** 85538-50-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 87.79 | kJ/mol | Joback Method |
| hf | -257.83 | kJ/mol | Joback Method |
| hfus | 20.37 | kJ/mol | Joback Method |
| hvap | 44.18 | kJ/mol | Joback Method |
| ie | 8.50 | eV | NIST Webbook |
| ie | 9.10 | eV | NIST Webbook |
| log10ws | -2.76 | | Crippen Method |
| logp | 2.848 | | Crippen Method |
| mcvol | 153.230 | ml/mol | McGowan Method |
| pc | 2467.81 | kPa | Joback Method |
| tb | 515.80 | K | Joback Method |
| tc | 729.04 | K | Joback Method |
| tf | 285.53 | K | Joback Method |
| vc | 0.579 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 398.11 | J/mol×K | 515.80 | Joback Method |
| cpg | 498.97 | J/mol×K | 693.50 | Joback Method |
| cpg | 481.29 | J/mol×K | 657.96 | Joback Method |
| cpg | 462.43 | J/mol×K | 622.42 | Joback Method |
| cpg | 442.33 | J/mol×K | 586.88 | Joback Method |
| cpg | 420.91 | J/mol×K | 551.34 | Joback Method |
| cpg | 515.56 | J/mol×K | 729.04 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0011714 | Pa×s | 515.80 | Joback Method |
| dvisc | 0.0011616 | Pa×s | 477.42 | Joback Method |
| dvisc | 0.0011503 | Pa×s | 439.04 | Joback Method |
| dvisc | 0.0011369 | Pa×s | 400.66 | Joback Method |
| dvisc | 0.0011208 | Pa×s | 362.29 | Joback Method |
| dvisc | 0.0011013 | Pa×s | 323.91 | Joback Method |
| dvisc | 0.0010770 | Pa×s | 285.53 | 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=C85538507&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 |
| **ie:** | Ionization energy |
| **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 |

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https://www.chemeo.com/cid/79-404-6/Tricyclo-4-3-1-1-2-5-undecane-10-methoxy-stereoisomer.pdf
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