# tricyclo[3.3.1.1(3,7)]decane-2-carboxylic acid, methyl ester

**Other names:** methyl tricyclo[3.3.1.1(3,7)]decane-2-carboxylate
Adamantane-2-carboxylic acid, methyl ester

**Inchi:** InChI=1S/C12H18O2/c1-14-12(13)11-9-3-7-2-8(5-9)6-10(11)4-7/h7-11H,2-6H2,1H3

**InchiKey:** IRGQVHHWSAJAFS-UHFFFAOYSA-N

**Formula:** C12H18O2

**SMILES:** COC(=O)C1C2CC3CC(C2)CC1C3

**Mol. weight [g/mol]:** 194.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -29.03 | kJ/mol | Joback Method |
| hf | -364.25 | kJ/mol | Joback Method |
| hfus | 24.07 | kJ/mol | Joback Method |
| hvap | 50.75 | kJ/mol | Joback Method |
| log10ws | -2.18 | | Crippen Method |
| logp | 2.232 | | Crippen Method |
| mcvol | 154.800 | ml/mol | McGowan Method |
| pc | 2563.69 | kPa | Joback Method |
| rinpol | 1494.00 | | NIST Webbook |
| rinpol | 1507.00 | | NIST Webbook |
| rinpol | 1467.00 | | NIST Webbook |
| rinpol | 1482.00 | | NIST Webbook |
| ripol | 1965.00 | | NIST Webbook |
| ripol | 1921.00 | | NIST Webbook |
| ripol | 1944.00 | | NIST Webbook |
| tb | 565.40 | K | Joback Method |
| tc | 779.60 | K | Joback Method |
| tf | 338.98 | K | Joback Method |
| vc | 0.593 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 426.54 | J/mol×K | 565.40 | Joback Method |

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|---|---|---|---|---|
| cpg | 446.47 | J/mol×K | 601.10 | Joback Method |
| cpg | 465.13 | J/mol×K | 636.80 | Joback Method |
| cpg | 482.59 | J/mol×K | 672.50 | Joback Method |
| cpg | 498.93 | J/mol×K | 708.20 | Joback Method |
| cpg | 514.23 | J/mol×K | 743.90 | Joback Method |
| cpg | 528.57 | J/mol×K | 779.60 | Joback Method |
| dvisc | 0.0020614 | Pa×s | 338.98 | Joback Method |
| dvisc | 0.0020742 | Pa×s | 376.72 | Joback Method |
| dvisc | 0.0020847 | Pa×s | 414.45 | Joback Method |
| dvisc | 0.0020935 | Pa×s | 452.19 | Joback Method |
| dvisc | 0.0021009 | Pa×s | 489.93 | Joback Method |
| dvisc | 0.0021074 | Pa×s | 527.66 | Joback Method |
| dvisc | 0.0021129 | Pa×s | 565.40 | Joback Method |

# Sources

| | |
|---|---|
| **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=U400307&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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