# Methyl dehydrogeraniate

**Inchi:** InChI=1S/C11H16O2/c1-9(2)6-5-7-10(3)8-11(12)13-4/h5-8H,1-4H3/b7-5+,10-8+
**InchiKey:** MUIMRDAQSNCVEQ-RMTFUQJTSA-N
**Formula:** C11H16O2
**SMILES:** COC(=O)C=C(C)C=CC=C(C)C
**Mol. weight [g/mol]:** 180.24
**CAS:** 53771-48-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 31.38 | kJ/mol | Joback Method |
| hf | -183.09 | kJ/mol | Joback Method |
| hfus | 25.02 | kJ/mol | Joback Method |
| hvap | 49.27 | kJ/mol | Joback Method |
| log10ws | -2.85 | | Crippen Method |
| logp | 2.628 | | Crippen Method |
| mcvol | 160.390 | ml/mol | McGowan Method |
| pc | 2351.92 | kPa | Joback Method |
| rinpol | 1475.30 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| rinpol | 1475.30 | | NIST Webbook |
| rinpol | 1445.00 | | NIST Webbook |
| tb | 539.61 | K | Joback Method |
| tc | 740.19 | K | Joback Method |
| tf | 242.73 | K | Joback Method |
| vc | 0.618 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 360.46 | J/mol×K | 539.61 | Joback Method |
| cpg | 374.67 | J/mol×K | 573.04 | Joback Method |
| cpg | 388.08 | J/mol×K | 606.47 | Joback Method |
| cpg | 400.75 | J/mol×K | 639.90 | Joback Method |
| cpg | 412.71 | J/mol×K | 673.33 | Joback Method |

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|---|---|---|---|---|
| cpg | 424.02 | J/mol×K | 706.76 | Joback Method |
| cpg | 434.72 | J/mol×K | 740.19 | 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=C53771485&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |