# Geranyl isohexanoate

**Inchi:** InChI=1S/C16H28O2/c1-13(2)7-6-8-15(5)11-12-18-16(17)10-9-14(3)4/h7,11,14H,6,8-10,
**InchiKey:** DUFDVHTVEPGEQM-PTNGSMBKSA-N
**Formula:** C16H28O2
**SMILES:** CC(C)=CCCC(C)=CCOC(=O)CCC(C)C
**Mol. weight [g/mol]:** 252.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -9.18 | kJ/mol | Joback Method |
| hf | -408.79 | kJ/mol | Joback Method |
| hfus | 34.24 | kJ/mol | Joback Method |
| hvap | 60.05 | kJ/mol | Joback Method |
| log10ws | -4.85 | | Crippen Method |
| logp | 4.659 | | Crippen Method |
| mcvol | 235.140 | ml/mol | McGowan Method |
| pc | 1495.35 | kPa | Joback Method |
| rinpol | 1681.00 | | NIST Webbook |
| rinpol | 1681.00 | | NIST Webbook |
| tb | 649.41 | K | Joback Method |
| tc | 834.76 | K | Joback Method |
| tf | 289.16 | K | Joback Method |
| vc | 0.911 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 633.96 | J/mol×K | 649.41 | Joback Method |
| cpg | 651.71 | J/mol×K | 680.30 | Joback Method |
| cpg | 668.60 | J/mol×K | 711.19 | Joback Method |
| cpg | 684.64 | J/mol×K | 742.09 | Joback Method |
| cpg | 699.90 | J/mol×K | 772.98 | Joback Method |
| cpg | 714.39 | J/mol×K | 803.87 | Joback Method |
| cpg | 728.16 | J/mol×K | 834.76 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R200672&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

# 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 |