# Benzenepropanoic acid, 3,7-dimethylocta-2,6-dienyl ester

**Other names:** geranyl 3-phenylpropanoate
**Inchi:** InChI=1S/C19H26O2/c1-16(2)8-7-9-17(3)14-15-21-19(20)13-12-18-10-5-4-6-11-18/h4-6,
**InchiKey:** RNXGADQWNZYSFZ-SAPNQHFASA-N
**Formula:** C19H26O2
**SMILES:** CC(C)=CCCC(C)=CCOC(=O)CCc1ccccc1
**Mol. weight [g/mol]:** 286.41
**CAS:** 74339-36-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 130.93 | kJ/mol | Joback Method |
| hf | -228.90 | kJ/mol | Joback Method |
| hfus | 39.58 | kJ/mol | Joback Method |
| hvap | 69.40 | kJ/mol | Joback Method |
| log10ws | -5.45 | | Crippen Method |
| logp | 4.855 | | Crippen Method |
| mcvol | 253.650 | ml/mol | McGowan Method |
| pc | 1536.66 | kPa | Joback Method |
| rinpol | 2125.00 | | NIST Webbook |
| rinpol | 2125.00 | | NIST Webbook |
| ripol | 2740.00 | | NIST Webbook |
| ripol | 2765.00 | | NIST Webbook |
| tb | 745.17 | K | Joback Method |
| tc | 952.83 | K | Joback Method |
| tf | 364.39 | K | Joback Method |
| vc | 0.978 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 719.77 | J/mol×K | 745.17 | Joback Method |
| cpg | 737.28 | J/mol×K | 779.78 | Joback Method |
| cpg | 753.73 | J/mol×K | 814.39 | Joback Method |
| cpg | 769.20 | J/mol×K | 849.00 | Joback Method |

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|---|---|---|---|---|
| cpg | 783.75 | J/mol×K | 883.61 | Joback Method |
| cpg | 797.45 | J/mol×K | 918.22 | Joback Method |
| cpg | 810.37 | J/mol×K | 952.83 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C74339369&Units=SI |

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