# Nerolidyl propionate

**Other names:** trans-nerolidyl propanoate
**Inchi:** InChI=1S/C18H30O2/c1-7-17(19)20-18(6,8-2)14-10-13-16(5)12-9-11-15(3)4/h8,11,13H,2
**InchiKey:** NPSBIIPKEQTFPA-SSZFMOIBSA-N
**Formula:** C18H30O2
**SMILES:** C=CC(C)(CCC=C(C)CCC=C(C)C)OC(=O)CC
**Mol. weight [g/mol]:** 278.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 100.78 | kJ/mol | Joback Method |
| hf | -328.11 | kJ/mol | Joback Method |
| hfus | 34.25 | kJ/mol | Joback Method |
| hvap | 62.93 | kJ/mol | Joback Method |
| log10ws | -5.89 | | Crippen Method |
| logp | 5.357 | | Crippen Method |
| mcvol | 259.020 | ml/mol | McGowan Method |
| pc | 1346.69 | kPa | Joback Method |
| rinpol | 1829.00 | | NIST Webbook |
| rinpol | 1850.00 | | NIST Webbook |
| rinpol | 1829.00 | | NIST Webbook |
| tb | 689.06 | K | Joback Method |
| tc | 879.50 | K | Joback Method |
| tf | 327.36 | K | Joback Method |
| vc | 1.000 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 723.33 | J/mol×K | 689.06 | Joback Method |
| cpg | 741.55 | J/mol×K | 720.80 | Joback Method |
| cpg | 758.80 | J/mol×K | 752.54 | Joback Method |
| cpg | 775.14 | J/mol×K | 784.28 | Joback Method |
| cpg | 790.61 | J/mol×K | 816.02 | Joback Method |
| cpg | 805.30 | J/mol×K | 847.76 | Joback Method |

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|---|---|---|---|---|
| cpg | 819.26 | J/mol×K | 879.50 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U132164&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 |

# 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 |