# Fumaric acid, nonyl pent-4-en-2-yl ester

**Inchi:** InChI=1S/C18H30O4/c1-4-6-7-8-9-10-11-15-21-17(19)13-14-18(20)22-16(3)12-5-2/h5,13
**InchiKey:** UAVIVXAGEACBPZ-BUHFOSPRSA-N
**Formula:** C18H30O4
**SMILES:** C=CCC(C)OC(=O)C=CC(=O)OCCCCCCCCC
**Mol. weight [g/mol]:** 310.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -201.54 | kJ/mol | Joback Method |
| hf | -667.08 | kJ/mol | Joback Method |
| hfus | 43.35 | kJ/mol | Joback Method |
| hvap | 72.87 | kJ/mol | Joback Method |
| log10ws | -4.90 | | Crippen Method |
| logp | 4.344 | | Crippen Method |
| mcvol | 270.760 | ml/mol | McGowan Method |
| pc | 1320.39 | kPa | Joback Method |
| rinpol | 2096.00 | | NIST Webbook |
| tb | 764.22 | K | Joback Method |
| tc | 949.22 | K | Joback Method |
| tf | 415.10 | K | Joback Method |
| vc | 1.046 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 799.90 | J/mol×K | 764.22 | Joback Method |
| cpg | 816.41 | J/mol×K | 795.05 | Joback Method |
| cpg | 832.01 | J/mol×K | 825.89 | Joback Method |
| cpg | 846.75 | J/mol×K | 856.72 | Joback Method |
| cpg | 860.63 | J/mol×K | 887.56 | Joback Method |
| cpg | 873.69 | J/mol×K | 918.39 | Joback Method |
| cpg | 885.95 | J/mol×K | 949.22 | Joback Method |
| dvisc | 0.0011583 | Pa×s | 415.10 | Joback Method |
| dvisc | 0.0005221 | Pa×s | 473.29 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002802 | Pa×s | 531.47 | Joback Method |
| dvisc | 0.0001700 | Pa×s | 589.66 | Joback Method |
| dvisc | 0.0001128 | Pa×s | 647.85 | Joback Method |
| dvisc | 0.0000801 | Pa×s | 706.03 | Joback Method |
| dvisc | 0.0000599 | Pa×s | 764.22 | 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=U348928&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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |