# Fumaric acid, heptyl 2-methylpentyl ester

**Inchi:** InChI=1S/C17H30O4/c1-4-6-7-8-9-13-20-16(18)11-12-17(19)21-14-15(3)10-5-2/h11-12,1
**InchiKey:** ODNOMTBXFJOGNC-VAWYXSNFSA-N
**Formula:** C17H30O4
**SMILES:** CCCCCCCOC(=O)C=CC(=O)OCC(C)CCC
**Mol. weight [g/mol]:** 298.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -297.80 | kJ/mol | Joback Method |
| hf | -771.87 | kJ/mol | Joback Method |
| hfus | 42.04 | kJ/mol | Joback Method |
| hvap | 71.32 | kJ/mol | Joback Method |
| log10ws | -4.28 | | Crippen Method |
| logp | 4.036 | | Crippen Method |
| mcvol | 260.970 | ml/mol | McGowan Method |
| pc | 1373.78 | kPa | Joback Method |
| rinpol | 1973.00 | | NIST Webbook |
| rinpol | 1973.00 | | NIST Webbook |
| tb | 744.66 | K | Joback Method |
| tc | 927.57 | K | Joback Method |
| tf | 405.59 | K | Joback Method |
| vc | 1.010 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 767.78 | J/mol×K | 744.66 | Joback Method |
| cpg | 784.43 | J/mol×K | 775.14 | Joback Method |
| cpg | 800.20 | J/mol×K | 805.63 | Joback Method |
| cpg | 815.12 | J/mol×K | 836.11 | Joback Method |
| cpg | 829.19 | J/mol×K | 866.60 | Joback Method |
| cpg | 842.44 | J/mol×K | 897.08 | Joback Method |
| cpg | 854.89 | J/mol×K | 927.57 | Joback Method |
| dvisc | 0.0012840 | Pa×s | 405.59 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005755 | Pa×s | 462.10 | Joback Method |
| dvisc | 0.0003072 | Pa×s | 518.61 | Joback Method |
| dvisc | 0.0001855 | Pa×s | 575.12 | Joback Method |
| dvisc | 0.0001226 | Pa×s | 631.64 | Joback Method |
| dvisc | 0.0000868 | Pa×s | 688.15 | Joback Method |
| dvisc | 0.0000647 | Pa×s | 744.66 | 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=U348726&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 |