# Fumaric acid, pentyl 2-propylphenyl ester

**Inchi:** InChI=1S/C18H24O4/c1-3-5-8-14-21-17(19)12-13-18(20)22-16-11-7-6-10-15(16)9-4-2/h6
**InchiKey:** PUUUUMCDWXMZSN-OUKQBFOZSA-N
**Formula:** C18H24O4
**SMILES:** CCCCCOC(=O)C=CC(=O)Oc1ccccc1CCC
**Mol. weight [g/mol]:** 304.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -184.16 | kJ/mol | Joback Method |
| hf | -562.17 | kJ/mol | Joback Method |
| hfus | 41.80 | kJ/mol | Joback Method |
| hvap | 76.87 | kJ/mol | Joback Method |
| log10ws | -4.65 | | Crippen Method |
| logp | 3.834 | | Crippen Method |
| mcvol | 251.300 | ml/mol | McGowan Method |
| pc | 1618.07 | kPa | Joback Method |
| rinpol | 2160.00 | | NIST Webbook |
| tb | 799.64 | K | Joback Method |
| tc | 1004.52 | K | Joback Method |
| tf | 470.80 | K | Joback Method |
| vc | 0.964 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 735.73 | J/mol×K | 799.64 | Joback Method |
| cpg | 750.91 | J/mol×K | 833.79 | Joback Method |
| cpg | 765.08 | J/mol×K | 867.93 | Joback Method |
| cpg | 778.26 | J/mol×K | 902.08 | Joback Method |
| cpg | 790.48 | J/mol×K | 936.23 | Joback Method |
| cpg | 801.78 | J/mol×K | 970.37 | Joback Method |
| cpg | 812.18 | J/mol×K | 1004.52 | Joback Method |
| dvisc | 0.0006620 | Pa×s | 470.80 | Joback Method |
| dvisc | 0.0003640 | Pa×s | 525.61 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002241 | Pa×s | 580.41 | Joback Method |
| dvisc | 0.0001500 | Pa×s | 635.22 | Joback Method |
| dvisc | 0.0001070 | Pa×s | 690.03 | Joback Method |
| dvisc | 0.0000803 | Pa×s | 744.83 | Joback Method |
| dvisc | 0.0000626 | Pa×s | 799.64 | 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=U348127&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **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 |

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