# Fumaric acid, 3-phenylpropyl 2-methylpent-3-yl ester

**Inchi:** InChI=1S/C19H26O4/c1-4-17(15(2)3)23-19(21)13-12-18(20)22-14-8-11-16-9-6-5-7-10-16

**InchiKey:** DSJOBIJGUVGHFM-OUKQBFOZSA-N

**Formula:** C19H26O4

**SMILES:** CCC(OC(=O)C=CC(=O)OCCCc1ccccc1)C(C)C

**Mol. weight [g/mol]:** 318.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -170.99 | kJ/mol | Joback Method |
| hf | -581.90 | kJ/mol | Joback Method |
| hfus | 37.74 | kJ/mol | Joback Method |
| hvap | 77.66 | kJ/mol | Joback Method |
| log10ws | -4.33 | | Crippen Method |
| logp | 3.696 | | Crippen Method |
| mcvol | 265.390 | ml/mol | McGowan Method |
| pc | 1536.66 | kPa | Joback Method |
| rinpol | 2271.00 | | NIST Webbook |
| tb | 816.66 | K | Joback Method |
| tc | 1024.80 | K | Joback Method |
| tf | 439.55 | K | Joback Method |
| vc | 1.008 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 794.92 | J/mol×K | 816.66 | Joback Method |
| cpg | 863.43 | J/mol×K | 990.11 | Joback Method |
| cpg | 851.81 | J/mol×K | 955.42 | Joback Method |
| cpg | 839.19 | J/mol×K | 920.73 | Joback Method |
| cpg | 825.52 | J/mol×K | 886.04 | Joback Method |
| cpg | 810.78 | J/mol×K | 851.35 | Joback Method |
| cpg | 874.09 | J/mol×K | 1024.80 | Joback Method |
| dvisc | 0.0000457 | Pa×s | 816.66 | Joback Method |
| dvisc | 0.0000615 | Pa×s | 753.81 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000875 | Pa×s | 690.96 | Joback Method |
| dvisc | 0.0001336 | Pa×s | 628.11 | Joback Method |
| dvisc | 0.0002241 | Pa×s | 565.25 | Joback Method |
| dvisc | 0.0004278 | Pa×s | 502.40 | Joback Method |
| dvisc | 0.0009825 | Pa×s | 439.55 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U405662&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 |
| **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 |