# Fumaric acid, 2,4,4-trimethylpentyl 2-methylpent-3-yl ester

**Inchi:** InChI=1S/C18H32O4/c1-8-15(13(2)3)22-17(20)10-9-16(19)21-12-14(4)11-18(5,6)7/h9-10

**InchiKey:** WDSSORKNQLETJT-MDZDMXLPSA-N

**Formula:** C18H32O4

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

**Mol. weight [g/mol]:** 312.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -291.42 | kJ/mol | Joback Method |
| hf | -811.82 | kJ/mol | Joback Method |
| hfus | 30.17 | kJ/mol | Joback Method |
| hvap | 71.47 | kJ/mol | Joback Method |
| log10ws | -4.32 | | Crippen Method |
| logp | 4.136 | | Crippen Method |
| mcvol | 275.060 | ml/mol | McGowan Method |
| pc | 1313.70 | kPa | Joback Method |
| rinpol | 1903.00 | | NIST Webbook |
| rinpol | 1903.00 | | NIST Webbook |
| tb | 763.43 | K | Joback Method |
| tc | 956.24 | K | Joback Method |
| tf | 389.28 | K | Joback Method |
| vc | 1.042 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 828.30 | J/mol×K | 763.43 | Joback Method |
| cpg | 906.50 | J/mol×K | 924.11 | Joback Method |
| cpg | 892.78 | J/mol×K | 891.97 | Joback Method |
| cpg | 878.13 | J/mol×K | 859.84 | Joback Method |
| cpg | 862.53 | J/mol×K | 827.70 | Joback Method |
| cpg | 845.93 | J/mol×K | 795.57 | Joback Method |
| cpg | 919.35 | J/mol×K | 956.24 | Joback Method |
| dvisc | 0.0000390 | Pa×s | 763.43 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000558 | Pa×s | 701.07 | Joback Method |
| dvisc | 0.0000856 | Pa×s | 638.71 | Joback Method |
| dvisc | 0.0001441 | Pa×s | 576.36 | Joback Method |
| dvisc | 0.0002750 | Pa×s | 514.00 | Joback Method |
| dvisc | 0.0006277 | Pa×s | 451.64 | Joback Method |
| dvisc | 0.0018664 | Pa×s | 389.28 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U405602&Units=SI |

# 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 |