# Fumaric acid, 2-methylpentyl 3-methylbut-2-yl ester

**Inchi:** InChI=1S/C15H26O4/c1-6-7-12(4)10-18-14(16)8-9-15(17)19-13(5)11(2)3/h8-9,11-13H,6-

**InchiKey:** DLRBWAPHIAZTHZ-CMDGGOBGSA-N

**Formula:** C15H26O4

**SMILES:** CCCC(C)COC(=O)C=CC(=O)OC(C)C(C)C

**Mol. weight [g/mol]:** 270.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -319.52 | kJ/mol | Joback Method |
| hf | -741.15 | kJ/mol | Joback Method |
| hfus | 29.81 | kJ/mol | Joback Method |
| hvap | 66.09 | kJ/mol | Joback Method |
| log10ws | -3.31 | | Crippen Method |
| logp | 3.110 | | Crippen Method |
| mcvol | 232.790 | ml/mol | McGowan Method |
| pc | 1612.88 | kPa | Joback Method |
| rinpol | 1740.00 | | NIST Webbook |
| tb | 698.02 | K | Joback Method |
| tc | 886.19 | K | Joback Method |
| tf | 353.05 | K | Joback Method |
| vc | 0.885 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 656.12 | J/mol×K | 698.02 | Joback Method |
| cpg | 672.46 | J/mol×K | 729.38 | Joback Method |
| cpg | 687.94 | J/mol×K | 760.74 | Joback Method |
| cpg | 702.57 | J/mol×K | 792.10 | Joback Method |
| cpg | 716.37 | J/mol×K | 823.46 | Joback Method |
| cpg | 729.35 | J/mol×K | 854.82 | Joback Method |
| cpg | 741.53 | J/mol×K | 886.19 | Joback Method |
| dvisc | 0.0025568 | Pa×s | 353.05 | Joback Method |
| dvisc | 0.0009302 | Pa×s | 410.55 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004338 | Pa×s | 468.04 | Joback Method |
| dvisc | 0.0002391 | Pa×s | 525.53 | Joback Method |
| dvisc | 0.0001482 | Pa×s | 583.03 | Joback Method |
| dvisc | 0.0001001 | Pa×s | 640.52 | Joback Method |
| dvisc | 0.0000721 | Pa×s | 698.02 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U405646&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |