# Fumaric acid, butyl 3-ethylphenyl ester

**Inchi:** InChI=1S/C16H20O4/c1-3-5-11-19-15(17)9-10-16(18)20-14-8-6-7-13(4-2)12-14/h6-10,12
**InchiKey:** GTZFJRUPSXQDPO-MDZDMXLPSA-N
**Formula:** C16H20O4
**SMILES:** CCCCOC(=O)C=CC(=O)Oc1cccc(CC)c1
**Mol. weight [g/mol]:** 276.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -201.00 | kJ/mol | Joback Method |
| hf | -520.89 | kJ/mol | Joback Method |
| hfus | 36.62 | kJ/mol | Joback Method |
| hvap | 72.42 | kJ/mol | Joback Method |
| log10ws | -3.82 | | Crippen Method |
| logp | 3.054 | | Crippen Method |
| mcvol | 223.120 | ml/mol | McGowan Method |
| pc | 1900.26 | kPa | Joback Method |
| rinpol | 2084.00 | | NIST Webbook |
| rinpol | 2084.00 | | NIST Webbook |
| tb | 753.88 | K | Joback Method |
| tc | 961.93 | K | Joback Method |
| tf | 448.26 | K | Joback Method |
| vc | 0.852 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 623.96 | J/mol×K | 753.88 | Joback Method |
| cpg | 687.57 | J/mol×K | 927.25 | Joback Method |
| cpg | 676.67 | J/mol×K | 892.58 | Joback Method |
| cpg | 664.89 | J/mol×K | 857.90 | Joback Method |
| cpg | 652.19 | J/mol×K | 823.23 | Joback Method |
| cpg | 638.55 | J/mol×K | 788.55 | Joback Method |
| cpg | 697.61 | J/mol×K | 961.93 | Joback Method |
| dvisc | 0.0000809 | Pa×s | 753.88 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001030 | Pa×s | 702.94 | Joback Method |
| dvisc | 0.0001362 | Pa×s | 652.01 | Joback Method |
| dvisc | 0.0001887 | Pa×s | 601.07 | Joback Method |
| dvisc | 0.0002779 | Pa×s | 550.13 | Joback Method |
| dvisc | 0.0004428 | Pa×s | 499.20 | Joback Method |
| dvisc | 0.0007844 | Pa×s | 448.26 | 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=U348159&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 |