# Fumaric acid, hexyl 2-hexyl ester

**Inchi:** InChI=1S/C16H28O4/c1-4-6-8-9-13-19-15(17)11-12-16(18)20-14(3)10-7-5-2/h11-12,14H
**InchiKey:** LBHUSNDGDLKQEC-VAWYXSNFSA-N
**Formula:** C16H28O4
**SMILES:** CCCCCCOC(=O)C=CC(=O)OC(C)CCCC
**Mol. weight [g/mol]:** 284.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -306.22 | kJ/mol | Joback Method |
| hf | -751.23 | kJ/mol | Joback Method |
| hfus | 39.45 | kJ/mol | Joback Method |
| hvap | 69.09 | kJ/mol | Joback Method |
| log10ws | -4.21 | | Crippen Method |
| logp | 3.788 | | Crippen Method |
| mcvol | 246.880 | ml/mol | McGowan Method |
| pc | 1477.02 | kPa | Joback Method |
| rinpol | 1910.00 | | NIST Webbook |
| tb | 721.78 | K | Joback Method |
| tc | 904.51 | K | Joback Method |
| tf | 394.32 | K | Joback Method |
| vc | 0.954 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 710.90 | J/mol×K | 721.78 | Joback Method |
| cpg | 727.17 | J/mol×K | 752.23 | Joback Method |
| cpg | 742.59 | J/mol×K | 782.69 | Joback Method |
| cpg | 757.19 | J/mol×K | 813.14 | Joback Method |
| cpg | 770.99 | J/mol×K | 843.60 | Joback Method |
| cpg | 783.99 | J/mol×K | 874.05 | Joback Method |
| cpg | 796.23 | J/mol×K | 904.51 | Joback Method |
| dvisc | 0.0014186 | Pa×s | 394.32 | Joback Method |
| dvisc | 0.0006427 | Pa×s | 448.90 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003457 | Pa×s | 503.47 | Joback Method |
| dvisc | 0.0002100 | Pa×s | 558.05 | Joback Method |
| dvisc | 0.0001394 | Pa×s | 612.63 | Joback Method |
| dvisc | 0.0000989 | Pa×s | 667.20 | Joback Method |
| dvisc | 0.0000739 | Pa×s | 721.78 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U348745&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

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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 |