# Fumaric acid, 2,4,4-trimethylpentyl cyclohexylmethyl ester

**Inchi:** InChI=1S/C19H32O4/c1-15(12-19(2,3)4)13-22-17(20)10-11-18(21)23-14-16-8-6-5-7-9-16

**InchiKey:** SSHKZDXEEYOEHQ-ZHACJKMWSA-N

**Formula:** C19H32O4

**SMILES:** CC(COC(=O)C=CC(=O)OCC1CCCCC1)CC(C)(C)C

**Mol. weight [g/mol]:** 324.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -253.67 | kJ/mol | Joback Method |
| hf | -767.58 | kJ/mol | Joback Method |
| hfus | 31.64 | kJ/mol | Joback Method |
| hvap | 74.90 | kJ/mol | Joback Method |
| log10ws | -4.52 | | Crippen Method |
| logp | 4.282 | | Crippen Method |
| mcvol | 278.290 | ml/mol | McGowan Method |
| pc | 1406.95 | kPa | Joback Method |
| rinpol | 2220.00 | | NIST Webbook |
| rinpol | 2220.00 | | NIST Webbook |
| tb | 806.74 | K | Joback Method |
| tc | 1015.16 | K | Joback Method |
| tf | 437.93 | K | Joback Method |
| vc | 1.044 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 882.10 | J/mol×K | 806.74 | Joback Method |
| cpg | 900.96 | J/mol×K | 841.48 | Joback Method |
| cpg | 918.49 | J/mol×K | 876.21 | Joback Method |
| cpg | 934.77 | J/mol×K | 910.95 | Joback Method |
| cpg | 949.83 | J/mol×K | 945.68 | Joback Method |
| cpg | 963.74 | J/mol×K | 980.42 | Joback Method |
| cpg | 976.55 | J/mol×K | 1015.16 | Joback Method |
| dvisc | 0.0011677 | Pa×s | 437.93 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004731 | Pa×s | 499.40 | Joback Method |
| dvisc | 0.0002336 | Pa×s | 560.87 | Joback Method |
| dvisc | 0.0001326 | Pa×s | 622.34 | Joback Method |
| dvisc | 0.0000834 | Pa×s | 683.80 | Joback Method |
| dvisc | 0.0000566 | Pa×s | 745.27 | Joback Method |
| dvisc | 0.0000407 | Pa×s | 806.74 | Joback Method |

# Sources

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|---|---|
| **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=U405608&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 |