# Fumaric acid, 2,4,4-trimethylpentyl 2,2,3,3-tetrafluoropropyl ester

**Inchi:** InChI=1S/C15H22F4O4/c1-10(7-14(2,3)4)8-22-11(20)5-6-12(21)23-9-15(18,19)13(16)17/

**InchiKey:** VCBPVEHYIFBMGW-AATRIKPKSA-N

**Formula:** C15H22F4O4

**SMILES:** CC(COC(=O)C=CC(=O)OCC(F)(F)C(F)F)CC(C)(C)C

**Mol. weight [g/mol]:** 342.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1090.64 | kJ/mol | Joback Method |
| hf | -1537.81 | kJ/mol | Joback Method |
| hfus | 30.83 | kJ/mol | Joback Method |
| hvap | 60.62 | kJ/mol | Joback Method |
| log10ws | -3.82 | | Crippen Method |
| logp | 3.602 | | Crippen Method |
| mcvol | 239.870 | ml/mol | McGowan Method |
| pc | 1434.80 | kPa | Joback Method |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| tb | 689.08 | K | Joback Method |
| tc | 865.41 | K | Joback Method |
| tf | 375.25 | K | Joback Method |
| vc | 0.942 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 691.98 | J/mol×K | 689.08 | Joback Method |
| cpg | 706.65 | J/mol×K | 718.47 | Joback Method |
| cpg | 720.47 | J/mol×K | 747.86 | Joback Method |
| cpg | 733.49 | J/mol×K | 777.25 | Joback Method |
| cpg | 745.74 | J/mol×K | 806.64 | Joback Method |
| cpg | 757.26 | J/mol×K | 836.03 | Joback Method |
| cpg | 768.09 | J/mol×K | 865.41 | 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=U405598&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 |
| **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 |