# Fumaric acid, monoamide, N,N-dimethyl-, 4-isopropoxyphenyl ester

**Inchi:** InChI=1S/C15H19NO4/c1-11(2)19-12-5-7-13(8-6-12)20-15(18)10-9-14(17)16(3)4/h5-11H

**InchiKey:** GSBUVGNPDVPIMO-MDZDMXLPSA-N

**Formula:** C15H19NO4

**SMILES:** CC(C)Oc1ccc(OC(=O)C=CC(=O)N(C)C)cc1

**Mol. weight [g/mol]:** 277.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -101.08 | kJ/mol | Joback Method |
| hf | -438.00 | kJ/mol | Joback Method |
| hfus | 33.53 | kJ/mol | Joback Method |
| hvap | 71.85 | kJ/mol | Joback Method |
| log10ws | -2.73 | | Crippen Method |
| logp | 2.024 | | Crippen Method |
| mcvol | 219.010 | ml/mol | McGowan Method |
| pc | 2081.22 | kPa | Joback Method |
| rinpol | 2266.00 | | NIST Webbook |
| rinpol | 2266.00 | | NIST Webbook |
| tb | 743.00 | K | Joback Method |
| tc | 954.53 | K | Joback Method |
| tf | 454.46 | K | Joback Method |
| vc | 0.807 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 609.95 | J/mol×K | 743.00 | Joback Method |
| cpg | 624.56 | J/mol×K | 778.26 | Joback Method |
| cpg | 638.17 | J/mol×K | 813.51 | Joback Method |
| cpg | 650.79 | J/mol×K | 848.77 | Joback Method |
| cpg | 662.47 | J/mol×K | 884.02 | Joback Method |
| cpg | 673.24 | J/mol×K | 919.28 | Joback Method |
| cpg | 683.14 | J/mol×K | 954.53 | 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=U357420&Units=SI |

# 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 |