# Dimethylmalonic acid, ethyl 2-isopropoxyphenyl ester

**Inchi:** InChI=1S/C16H22O5/c1-6-19-14(17)16(4,5)15(18)21-13-10-8-7-9-12(13)20-11(2)3/h7-11
**InchiKey:** QKPGUWLSJSQVEX-UHFFFAOYSA-N
**Formula:** C16H22O5
**SMILES:** CCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
**Mol. weight [g/mol]:** 294.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -385.82 | kJ/mol | Joback Method |
| hf | -784.36 | kJ/mol | Joback Method |
| hfus | 26.67 | kJ/mol | Joback Method |
| hvap | 73.19 | kJ/mol | Joback Method |
| log10ws | -3.57 | | Crippen Method |
| logp | 2.968 | | Crippen Method |
| mcvol | 233.290 | ml/mol | McGowan Method |
| pc | 1832.54 | kPa | Joback Method |
| rinpol | 1817.00 | | NIST Webbook |
| tb | 768.47 | K | Joback Method |
| tc | 980.68 | K | Joback Method |
| tf | 462.99 | K | Joback Method |
| vc | 0.873 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 678.78 | J/mol×K | 768.47 | Joback Method |
| cpg | 694.04 | J/mol×K | 803.84 | Joback Method |
| cpg | 708.17 | J/mol×K | 839.21 | Joback Method |
| cpg | 721.20 | J/mol×K | 874.57 | Joback Method |
| cpg | 733.14 | J/mol×K | 909.94 | Joback Method |
| cpg | 744.02 | J/mol×K | 945.31 | Joback Method |
| cpg | 753.83 | J/mol×K | 980.68 | Joback Method |
| dvisc | 0.0006638 | Pa×s | 462.99 | Joback Method |
| dvisc | 0.0003542 | Pa×s | 513.90 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002116 | Pa×s | 564.82 | Joback Method |
| dvisc | 0.0001377 | Pa×s | 615.73 | Joback Method |
| dvisc | 0.0000956 | Pa×s | 666.64 | Joback Method |
| dvisc | 0.0000700 | Pa×s | 717.56 | Joback Method |
| dvisc | 0.0000534 | Pa×s | 768.47 | Joback Method |

# Sources

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|---|---|
| **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=U361849&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |