# Dimethylmalonic acid, 2-isopropoxyphenyl tetradecyl ester

**Inchi:** InChI=1S/C28H46O5/c1-6-7-8-9-10-11-12-13-14-15-16-19-22-31-26(29)28(4,5)27(30)33-
**InchiKey:** URQLQPIFNIOTHG-UHFFFAOYSA-N
**Formula:** C28H46O5
**SMILES:** CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
**Mol. weight [g/mol]:** 462.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -284.78 | kJ/mol | Joback Method |
| hf | -1032.04 | kJ/mol | Joback Method |
| hfus | 57.75 | kJ/mol | Joback Method |
| hvap | 99.90 | kJ/mol | Joback Method |
| log10ws | -8.59 | | Crippen Method |
| logp | 7.650 | | Crippen Method |
| mcvol | 402.370 | ml/mol | McGowan Method |
| pc | 821.95 | kPa | Joback Method |
| rinpol | 2970.00 | | NIST Webbook |
| tb | 1043.03 | K | Joback Method |
| tc | 1280.08 | K | Joback Method |
| tf | 598.23 | K | Joback Method |
| vc | 1.544 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1398.64 | J/mol×K | 1043.03 | Joback Method |
| cpg | 1415.74 | J/mol×K | 1082.54 | Joback Method |
| cpg | 1431.02 | J/mol×K | 1122.05 | Joback Method |
| cpg | 1444.57 | J/mol×K | 1161.55 | Joback Method |
| cpg | 1456.47 | J/mol×K | 1201.06 | Joback Method |
| cpg | 1466.78 | J/mol×K | 1240.57 | Joback Method |
| cpg | 1475.59 | J/mol×K | 1280.08 | Joback Method |
| dvisc | 0.0001510 | Pa×s | 598.23 | Joback Method |
| dvisc | 0.0000714 | Pa×s | 672.36 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000392 | Pa×s | 746.50 | Joback Method |
| dvisc | 0.0000239 | Pa×s | 820.63 | Joback Method |
| dvisc | 0.0000159 | Pa×s | 894.76 | Joback Method |
| dvisc | 0.0000112 | Pa×s | 968.90 | Joback Method |
| dvisc | 0.0000083 | Pa×s | 1043.03 | 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=U361862&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 |
| **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 |