# Dodecanoic acid, 2,3-dimethylphenyl ester

**Inchi:** InChI=1S/C20H32O2/c1-4-5-6-7-8-9-10-11-12-16-20(21)22-19-15-13-14-17(2)18(19)3/h1
**InchiKey:** FGJCENRKFKUYPW-UHFFFAOYSA-N
**Formula:** C20H32O2
**SMILES:** CCCCCCCCCCCC(=O)Oc1cccc(C)c1C
**Mol. weight [g/mol]:** 304.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -23.25 | kJ/mol | Joback Method |
| hf | -487.34 | kJ/mol | Joback Method |
| hfus | 43.61 | kJ/mol | Joback Method |
| hvap | 72.87 | kJ/mol | Joback Method |
| log10ws | -6.92 | | Crippen Method |
| logp | 6.130 | | Crippen Method |
| mcvol | 276.340 | ml/mol | McGowan Method |
| pc | 1283.75 | kPa | Joback Method |
| rinpol | 2332.00 | | NIST Webbook |
| tb | 769.93 | K | Joback Method |
| tc | 962.18 | K | Joback Method |
| tf | 438.78 | K | Joback Method |
| vc | 1.071 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 825.82 | J/mol×K | 769.93 | Joback Method |
| cpg | 843.91 | J/mol×K | 801.97 | Joback Method |
| cpg | 860.97 | J/mol×K | 834.01 | Joback Method |
| cpg | 877.05 | J/mol×K | 866.06 | Joback Method |
| cpg | 892.15 | J/mol×K | 898.10 | Joback Method |
| cpg | 906.31 | J/mol×K | 930.14 | Joback Method |
| cpg | 919.56 | J/mol×K | 962.18 | Joback Method |
| dvisc | 0.0008629 | Pa×s | 438.78 | Joback Method |
| dvisc | 0.0004574 | Pa×s | 493.97 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002754 | Pa×s | 549.16 | Joback Method |
| dvisc | 0.0001820 | Pa×s | 604.36 | Joback Method |
| dvisc | 0.0001289 | Pa×s | 659.55 | Joback Method |
| dvisc | 0.0000962 | Pa×s | 714.74 | Joback Method |
| dvisc | 0.0000749 | Pa×s | 769.93 | 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=U360547&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 |

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