# Myristic acid, 3-methylphenyl ester

**Inchi:** InChI=1S/C21H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-17-21(22)23-20-16-14-15-19(2)18-20
**InchiKey:** JDEVARUXESBALF-UHFFFAOYSA-N
**Formula:** C21H34O2
**SMILES:** CCCCCCCCCCCCCC(=O)Oc1cccc(C)c1
**Mol. weight [g/mol]:** 318.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -5.20 | kJ/mol | Joback Method |
| hf | -496.51 | kJ/mol | Joback Method |
| hfus | 46.58 | kJ/mol | Joback Method |
| hvap | 74.43 | kJ/mol | Joback Method |
| log10ws | -7.28 | | Crippen Method |
| logp | 6.602 | | Crippen Method |
| mcvol | 290.430 | ml/mol | McGowan Method |
| pc | 1212.36 | kPa | Joback Method |
| rinpol | 2418.00 | | NIST Webbook |
| tb | 787.83 | K | Joback Method |
| tc | 979.38 | K | Joback Method |
| tf | 437.53 | K | Joback Method |
| vc | 1.127 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 885.17 | J/mol×K | 787.83 | Joback Method |
| cpg | 967.02 | J/mol×K | 947.45 | Joback Method |
| cpg | 952.64 | J/mol×K | 915.53 | Joback Method |
| cpg | 937.30 | J/mol×K | 883.60 | Joback Method |
| cpg | 920.96 | J/mol×K | 851.68 | Joback Method |
| cpg | 903.60 | J/mol×K | 819.75 | Joback Method |
| cpg | 980.48 | J/mol×K | 979.38 | Joback Method |
| dvisc | 0.0000654 | Pa×s | 787.83 | Joback Method |
| dvisc | 0.0000854 | Pa×s | 729.45 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001170 | Pa×s | 671.06 | Joback Method |
| dvisc | 0.0001702 | Pa×s | 612.68 | Joback Method |
| dvisc | 0.0002679 | Pa×s | 554.30 | Joback Method |
| dvisc | 0.0004692 | Pa×s | 495.91 | Joback Method |
| dvisc | 0.0009543 | Pa×s | 437.53 | Joback Method |

# Sources

| | |
|---|---|
| **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=U357929&Units=SI |

# 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 |