# Cyclopropanecarboxylic acid, trans-2-phenyl-, tridec-4-yl ester

**Inchi:** InChI=1S/C23H36O2/c1-3-5-6-7-8-9-13-17-20(14-4-2)25-23(24)22-18-21(22)19-15-11-10

**InchiKey:** HFSYJZHPSQCRJU-UHFFFAOYSA-N

**Formula:** C23H36O2

**SMILES:** CCCCCCCCCC(CCC)OC(=O)C1CC1c1ccccc1

**Mol. weight [g/mol]:** 344.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 71.87 | kJ/mol | Joback Method |
| hf | -479.14 | kJ/mol | Joback Method |
| hfus | 47.84 | kJ/mol | Joback Method |
| hvap | 77.44 | kJ/mol | Joback Method |
| log10ws | -7.14 | | Crippen Method |
| logp | 6.643 | | Crippen Method |
| mcvol | 307.750 | ml/mol | McGowan Method |
| pc | 1153.78 | kPa | Joback Method |
| rinpol | 2470.00 | | NIST Webbook |
| rinpol | 2470.00 | | NIST Webbook |
| tb | 830.24 | K | Joback Method |
| tc | 1030.19 | K | Joback Method |
| tf | 446.25 | K | Joback Method |
| vc | 1.190 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 993.90 | J/mol×K | 830.24 | Joback Method |
| cpg | 1080.47 | J/mol×K | 996.87 | Joback Method |
| cpg | 1065.26 | J/mol×K | 963.54 | Joback Method |
| cpg | 1049.07 | J/mol×K | 930.22 | Joback Method |
| cpg | 1031.82 | J/mol×K | 896.89 | Joback Method |
| cpg | 1013.46 | J/mol×K | 863.57 | Joback Method |
| cpg | 1094.75 | J/mol×K | 1030.19 | Joback Method |
| dvisc | 0.0001771 | Pa×s | 830.24 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002199 | Pa×s | 766.24 | Joback Method |
| dvisc | 0.0002841 | Pa×s | 702.24 | Joback Method |
| dvisc | 0.0003863 | Pa×s | 638.25 | Joback Method |
| dvisc | 0.0005625 | Pa×s | 574.25 | Joback Method |
| dvisc | 0.0009001 | Pa×s | 510.25 | Joback Method |
| dvisc | 0.0016481 | Pa×s | 446.25 | Joback Method |

# Sources

| | |
|---|---|
| **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=U406251&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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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