# Hexanoic acid, 3,5,5-trimethyl-, pentadec-2-yl ester

**Inchi:** InChI=1S/C24H48O2/c1-7-8-9-10-11-12-13-14-15-16-17-18-22(3)26-23(25)19-21(2)20-2

**InchiKey:** QWXUBDGYOJQHIO-UHFFFAOYSA-N

**Formula:** C24H48O2

**SMILES:** CCCCCCCCCCCCCC(C)OC(=O)CC(C)CC(C)(C)C

**Mol. weight [g/mol]:** 368.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -84.76 | kJ/mol | Joback Method |
| hf | -802.80 | kJ/mol | Joback Method |
| hfus | 46.24 | kJ/mol | Joback Method |
| hvap | 76.10 | kJ/mol | Joback Method |
| log10ws | -8.36 | | Crippen Method |
| logp | 8.082 | | Crippen Method |
| mcvol | 356.460 | ml/mol | McGowan Method |
| pc | 844.56 | kPa | Joback Method |
| rinpol | 2336.00 | | NIST Webbook |
| rinpol | 2336.00 | | NIST Webbook |
| tb | 820.70 | K | Joback Method |
| tc | 1006.64 | K | Joback Method |
| tf | 404.82 | K | Joback Method |
| vc | 1.381 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1158.15 | J/mol×K | 820.70 | Joback Method |
| cpg | 1254.76 | J/mol×K | 975.65 | Joback Method |
| cpg | 1237.59 | J/mol×K | 944.66 | Joback Method |
| cpg | 1219.39 | J/mol×K | 913.67 | Joback Method |
| cpg | 1200.12 | J/mol×K | 882.68 | Joback Method |
| cpg | 1179.72 | J/mol×K | 851.69 | Joback Method |
| cpg | 1270.97 | J/mol×K | 1006.64 | Joback Method |
| dvisc | 0.0000281 | Pa×s | 820.70 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000404 | Pa×s | 751.39 | Joback Method |
| dvisc | 0.0000628 | Pa×s | 682.07 | Joback Method |
| dvisc | 0.0001078 | Pa×s | 612.76 | Joback Method |
| dvisc | 0.0002122 | Pa×s | 543.45 | Joback Method |
| dvisc | 0.0005093 | Pa×s | 474.13 | Joback Method |
| dvisc | 0.0016496 | Pa×s | 404.82 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406272&Units=SI |
| **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 |

# 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 |