# Hexanoic acid, 3,5,5-trimethyl-, tetradecyl ester

**Inchi:** InChI=1S/C23H46O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-25-22(24)19-21(2)20-23(3

**InchiKey:** KUGGOUVGKCLGGH-UHFFFAOYSA-N

**Formula:** C23H46O2

**SMILES:** CCCCCCCCCCCCCCOC(=O)CC(C)CC(C)(C)C

**Mol. weight [g/mol]:** 354.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -90.74 | kJ/mol | Joback Method |
| hf | -776.88 | kJ/mol | Joback Method |
| hfus | 47.18 | kJ/mol | Joback Method |
| hvap | 74.26 | kJ/mol | Joback Method |
| log10ws | -7.83 | | Crippen Method |
| logp | 7.693 | | Crippen Method |
| mcvol | 342.370 | ml/mol | McGowan Method |
| pc | 889.47 | kPa | Joback Method |
| rinpol | 2340.00 | | NIST Webbook |
| rinpol | 2340.00 | | NIST Webbook |
| tb | 798.26 | K | Joback Method |
| tc | 980.37 | K | Joback Method |
| tf | 408.55 | K | Joback Method |
| vc | 1.331 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1094.71 | J/mol×K | 798.26 | Joback Method |
| cpg | 1189.55 | J/mol×K | 950.02 | Joback Method |
| cpg | 1172.62 | J/mol×K | 919.66 | Joback Method |
| cpg | 1154.71 | J/mol×K | 889.31 | Joback Method |
| cpg | 1135.79 | J/mol×K | 858.96 | Joback Method |
| cpg | 1115.80 | J/mol×K | 828.61 | Joback Method |
| cpg | 1205.56 | J/mol×K | 980.37 | Joback Method |
| dvisc | 0.0000357 | Pa×s | 798.26 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000505 | Pa×s | 733.31 | Joback Method |
| dvisc | 0.0000763 | Pa×s | 668.36 | Joback Method |
| dvisc | 0.0001262 | Pa×s | 603.40 | Joback Method |
| dvisc | 0.0002356 | Pa×s | 538.45 | Joback Method |
| dvisc | 0.0005220 | Pa×s | 473.50 | Joback Method |
| dvisc | 0.0014893 | Pa×s | 408.55 | Joback Method |

# Sources

| | |
|---|---|
| **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=U406065&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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