# Hexadecanoic acid, 2-hydroxy-15-methyl, methyl ester

**Inchi:** InChI=1S/C18H36O3/c1-16(2)14-12-10-8-6-4-5-7-9-11-13-15-17(19)18(20)21-3/h16-17,1

**InchiKey:** IKISEVPXUQJNRH-UHFFFAOYSA-N

**Formula:** C18H36O3

**SMILES:** COC(=O)C(O)CCCCCCCCCCCCC(C)C

**Mol. weight [g/mol]:** 300.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -274.94 | kJ/mol | Joback Method |
| hf | -822.44 | kJ/mol | Joback Method |
| hfus | 42.20 | kJ/mol | Joback Method |
| hvap | 80.72 | kJ/mol | Joback Method |
| log10ws | -5.35 | | Crippen Method |
| logp | 4.858 | | Crippen Method |
| mcvol | 277.790 | ml/mol | McGowan Method |
| pc | 1282.83 | kPa | Joback Method |
| rinpol | 2109.00 | | NIST Webbook |
| rinpol | 2089.00 | | NIST Webbook |
| rinpol | 2089.00 | | NIST Webbook |
| rinpol | 2109.00 | | NIST Webbook |
| tb | 778.83 | K | Joback Method |
| tc | 956.64 | K | Joback Method |
| tf | 395.60 | K | Joback Method |
| vc | 1.075 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 867.49 | J/mol×K | 778.83 | Joback Method |
| cpg | 884.65 | J/mol×K | 808.46 | Joback Method |
| cpg | 900.92 | J/mol×K | 838.10 | Joback Method |
| cpg | 916.33 | J/mol×K | 867.73 | Joback Method |
| cpg | 930.91 | J/mol×K | 897.37 | Joback Method |
| cpg | 944.67 | J/mol×K | 927.00 | Joback Method |

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|---|---|---|---|---|
| cpg | 957.64 | J/mol×K | 956.64 | Joback Method |
| dvisc | 0.0026782 | Pa×s | 395.60 | Joback Method |
| dvisc | 0.0006189 | Pa×s | 459.47 | Joback Method |
| dvisc | 0.0002045 | Pa×s | 523.34 | Joback Method |
| dvisc | 0.0000860 | Pa×s | 587.22 | Joback Method |
| dvisc | 0.0000429 | Pa×s | 651.09 | Joback Method |
| dvisc | 0.0000242 | Pa×s | 714.96 | Joback Method |
| dvisc | 0.0000150 | Pa×s | 778.83 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R98127&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 |

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