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

**Inchi:** InChI=1S/C20H40O2/c1-6-7-8-9-10-11-12-13-14-15-22-19(21)16-18(2)17-20(3,4)5/h18H
**InchiKey:** NAKCAHXAFQJWPH-UHFFFAOYSA-N
**Formula:** C20H40O2
**SMILES:** CCCCCCCCCCCOC(=O)CC(C)CC(C)(C)C
**Mol. weight [g/mol]:** 312.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -116.00 | kJ/mol | Joback Method |
| hf | -714.96 | kJ/mol | Joback Method |
| hfus | 39.41 | kJ/mol | Joback Method |
| hvap | 67.59 | kJ/mol | Joback Method |
| log10ws | -6.57 | | Crippen Method |
| logp | 6.523 | | Crippen Method |
| mcvol | 300.100 | ml/mol | McGowan Method |
| pc | 1064.48 | kPa | Joback Method |
| rinpol | 2037.00 | | NIST Webbook |
| rinpol | 2037.00 | | NIST Webbook |
| tb | 729.62 | K | Joback Method |
| tc | 906.03 | K | Joback Method |
| tf | 374.74 | K | Joback Method |
| vc | 1.163 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 910.48 | J/mol×K | 729.62 | Joback Method |
| cpg | 1001.18 | J/mol×K | 876.63 | Joback Method |
| cpg | 984.89 | J/mol×K | 847.23 | Joback Method |
| cpg | 967.71 | J/mol×K | 817.83 | Joback Method |
| cpg | 949.60 | J/mol×K | 788.42 | Joback Method |
| cpg | 930.54 | J/mol×K | 759.02 | Joback Method |
| cpg | 1016.62 | J/mol×K | 906.03 | Joback Method |
| dvisc | 0.0000560 | Pa×s | 729.62 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000790 | Pa×s | 670.47 | Joback Method |
| dvisc | 0.0001190 | Pa×s | 611.33 | Joback Method |
| dvisc | 0.0001958 | Pa×s | 552.18 | Joback Method |
| dvisc | 0.0003629 | Pa×s | 493.03 | Joback Method |
| dvisc | 0.0007958 | Pa×s | 433.89 | Joback Method |
| dvisc | 0.0022363 | Pa×s | 374.74 | 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=U406062&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