# Undec-10-ynoic acid, octyl ester

**Inchi:** InChI=1S/C19H34O2/c1-3-5-7-9-11-12-13-15-17-19(20)21-18-16-14-10-8-6-4-2/h1H,4-18
**InchiKey:** NFJBMLOIHOFIOS-UHFFFAOYSA-N
**Formula:** C19H34O2
**SMILES:** C#CCCCCCCCCC(=O)OCCCCCCCC
**Mol. weight [g/mol]:** 294.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 98.25 | kJ/mol | Joback Method |
| hf | -388.39 | kJ/mol | Joback Method |
| hfus | 50.73 | kJ/mol | Joback Method |
| hvap | 66.90 | kJ/mol | Joback Method |
| log10ws | -6.43 | | Crippen Method |
| logp | 5.644 | | Crippen Method |
| mcvol | 277.410 | ml/mol | McGowan Method |
| pc | 1232.88 | kPa | Joback Method |
| rinpol | 2011.00 | | NIST Webbook |
| rinpol | 2011.00 | | NIST Webbook |
| tb | 700.53 | K | Joback Method |
| tc | 874.48 | K | Joback Method |
| tf | 423.02 | K | Joback Method |
| vc | 1.085 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 798.07 | J/mol×K | 700.53 | Joback Method |
| cpg | 816.36 | J/mol×K | 729.52 | Joback Method |
| cpg | 833.80 | J/mol×K | 758.51 | Joback Method |
| cpg | 850.42 | J/mol×K | 787.51 | Joback Method |
| cpg | 866.23 | J/mol×K | 816.50 | Joback Method |
| cpg | 881.28 | J/mol×K | 845.49 | Joback Method |
| cpg | 895.57 | J/mol×K | 874.48 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406161&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |