# 1-Heneicosyl formate

**Inchi:** InChI=1S/C22H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-22-23
**InchiKey:** ZMGJNJFHZNMVCW-UHFFFAOYSA-N
**Formula:** C22H44O2
**SMILES:** CCCCCCCCCCCCCCCCCCCCCOC=O
**Mol. weight [g/mol]:** 340.58
**CAS:** 77899-03-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -70.16 | kJ/mol | Joback Method |
| hf | -715.21 | kJ/mol | Joback Method |
| hfus | 56.21 | kJ/mol | Joback Method |
| hvap | 73.70 | kJ/mol | Joback Method |
| log10ws | -7.89 | | Crippen Method |
| logp | 7.591 | | Crippen Method |
| mcvol | 328.280 | ml/mol | McGowan Method |
| pc | 933.49 | kPa | Joback Method |
| tb | 773.84 | K | Joback Method |
| tc | 948.88 | K | Joback Method |
| tf | 401.93 | K | Joback Method |
| vc | 1.302 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1029.43 | J/mol×K | 773.84 | Joback Method |
| cpg | 1049.93 | J/mol×K | 803.01 | Joback Method |
| cpg | 1069.43 | J/mol×K | 832.19 | Joback Method |
| cpg | 1087.96 | J/mol×K | 861.36 | Joback Method |
| cpg | 1105.55 | J/mol×K | 890.53 | Joback Method |
| cpg | 1122.22 | J/mol×K | 919.70 | Joback Method |
| cpg | 1138.00 | J/mol×K | 948.88 | Joback Method |
| dvisc | 0.0015648 | Pa×s | 401.93 | Joback Method |
| dvisc | 0.0006385 | Pa×s | 463.91 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0003218 | Pa×s | 525.90 | Joback Method |
| dvisc | 0.0001874 | Pa×s | 587.88 | Joback Method |
| dvisc | 0.0001210 | Pa×s | 649.87 | Joback Method |
| dvisc | 0.0000843 | Pa×s | 711.85 | Joback Method |
| dvisc | 0.0000622 | Pa×s | 773.84 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C77899037&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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