# 4-Heneicosanone, 1-cyclopentyl-

**Inchi:** InChI=1S/C26H50O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-26(27)24-19-22-25-20-
**InchiKey:** MEDPYMMZEVIBCH-UHFFFAOYSA-N
**Formula:** C26H50O
**SMILES:** CCCCCCCCCCCCCCCCCCC(=O)CCCC1CCCC1
**Mol. weight [g/mol]:** 378.67
**CAS:** 56247-96-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 75.67 | kJ/mol | Joback Method |
| hf | -632.07 | kJ/mol | Joback Method |
| hfus | 58.63 | kJ/mol | Joback Method |
| hvap | 80.47 | kJ/mol | Joback Method |
| log10ws | -9.64 | | Crippen Method |
| logp | 9.178 | | Crippen Method |
| mcvol | 367.910 | ml/mol | McGowan Method |
| pc | 830.02 | kPa | Joback Method |
| tb | 863.43 | K | Joback Method |
| tc | 1057.55 | K | Joback Method |
| tf | 326.65 ± 2.00 | K | NIST Webbook |
| vc | 1.438 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1245.45 | J/mol×K | 863.43 | Joback Method |
| cpg | 1268.19 | J/mol×K | 895.78 | Joback Method |
| cpg | 1289.64 | J/mol×K | 928.14 | Joback Method |
| cpg | 1309.87 | J/mol×K | 960.49 | Joback Method |
| cpg | 1328.94 | J/mol×K | 992.85 | Joback Method |
| cpg | 1346.92 | J/mol×K | 1025.20 | Joback Method |
| cpg | 1363.88 | J/mol×K | 1057.55 | Joback Method |
| dvisc | 0.0015282 | Pa×s | 443.61 | Joback Method |
| dvisc | 0.0006242 | Pa×s | 513.58 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003160 | Pa×s | 583.55 | Joback Method |
| dvisc | 0.0001851 | Pa×s | 653.52 | Joback Method |
| dvisc | 0.0001202 | Pa×s | 723.49 | Joback Method |
| dvisc | 0.0000843 | Pa×s | 793.46 | Joback Method |
| dvisc | 0.0000626 | Pa×s | 863.43 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C56247962&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 |