# 2-Hexanone, 1,1,1,3,3-d5-

**Inchi:** InChI=1S/C6H12O/c1-3-4-5-6(2)7/h3-5H2,1-2H3/i2D3,5D2
**InchiKey:** QQZOPKMRPOGIEB-ZTIZGVCASA-N
**Formula:** C6H7D5O
**SMILES:** CCCCC(C)=O
**Mol. weight [g/mol]:** 105.19
**CAS:** 4840-82-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -129.28 | kJ/mol | Joback Method |
| hf | -279.75 | kJ/mol | Joback Method |
| hfus | 12.89 | kJ/mol | Joback Method |
| hvap | 35.70 | kJ/mol | Joback Method |
| log10ws | -1.61 | | Crippen Method |
| logp | 1.766 | | Crippen Method |
| mcvol | 96.970 | ml/mol | McGowan Method |
| pc | 3337.38 | kPa | Joback Method |
| tb | 390.55 | K | Joback Method |
| tc | 568.08 | K | Joback Method |
| tf | 207.31 | K | Joback Method |
| vc | 0.378 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 177.72 | J/mol×K | 390.55 | Joback Method |
| cpg | 187.80 | J/mol×K | 420.14 | Joback Method |
| cpg | 197.51 | J/mol×K | 449.73 | Joback Method |
| cpg | 206.83 | J/mol×K | 479.31 | Joback Method |
| cpg | 215.79 | J/mol×K | 508.90 | Joback Method |
| cpg | 224.39 | J/mol×K | 538.49 | Joback Method |
| cpg | 232.63 | J/mol×K | 568.08 | Joback Method |
| dvisc | 0.0038104 | Pa×s | 207.31 | Joback Method |
| dvisc | 0.0019023 | Pa×s | 237.85 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0011124 | Pa×s | 268.39 | Joback Method |
| dvisc | 0.0007258 | Pa×s | 298.93 | Joback Method |
| dvisc | 0.0005126 | Pa×s | 329.47 | Joback Method |
| dvisc | 0.0003840 | Pa×s | 360.01 | Joback Method |
| dvisc | 0.0003010 | Pa×s | 390.55 | 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=C4840828&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |