# 2-Heptyne, 5-methyl

**Inchi:** InChI=1S/C8H14/c1-4-6-7-8(3)5-2/h8H,5,7H2,1-3H3
**InchiKey:** IBUAQOAHFNAARK-UHFFFAOYSA-N
**Formula:** C8H14
**SMILES:** CC#CCC(C)CC
**Mol. weight [g/mol]:** 110.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 216.84 | kJ/mol | Joback Method |
| hf | 58.57 | kJ/mol | Joback Method |
| hfus | 16.07 | kJ/mol | Joback Method |
| hvap | 35.17 | kJ/mol | Joback Method |
| log10ws | -2.72 | | Crippen Method |
| logp | 2.446 | | Crippen Method |
| mcvol | 114.980 | ml/mol | McGowan Method |
| pc | 3025.61 | kPa | Joback Method |
| rinpol | 811.00 | | NIST Webbook |
| rinpol | 811.00 | | NIST Webbook |
| tb | 391.00 | K | Joback Method |
| tc | 582.81 | K | Joback Method |
| tf | 271.02 | K | Joback Method |
| vc | 0.440 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 208.33 | J/mol×K | 391.00 | Joback Method |
| cpg | 220.75 | J/mol×K | 422.97 | Joback Method |
| cpg | 232.68 | J/mol×K | 454.94 | Joback Method |
| cpg | 244.12 | J/mol×K | 486.91 | Joback Method |
| cpg | 255.09 | J/mol×K | 518.88 | Joback Method |
| cpg | 265.59 | J/mol×K | 550.85 | Joback Method |
| cpg | 275.65 | J/mol×K | 582.81 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R66554&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

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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 |