# 3-hexyl-2,5-dimethyl-5,6-dihydropyrazine

**Inchi:** InChI=1S/C12H22N2/c1-4-5-6-7-8-12-11(3)13-9-10(2)14-12/h10H,4-9H2,1-3H3
**InchiKey:** CGSGWEMRCJYHEC-UHFFFAOYSA-N
**Formula:** C12H22N2
**SMILES:** CCCCCCC1=NC(C)CN=C1C
**Mol. weight [g/mol]:** 194.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 348.83 | kJ/mol | Joback Method |
| hf | -2.13 | kJ/mol | Joback Method |
| hfus | 30.61 | kJ/mol | Joback Method |
| hvap | 57.06 | kJ/mol | Joback Method |
| log10ws | -3.18 | | Crippen Method |
| logp | 3.261 | | Crippen Method |
| mcvol | 180.440 | ml/mol | McGowan Method |
| pc | 2222.89 | kPa | Joback Method |
| rinpol | 1380.00 | | NIST Webbook |
| tb | 609.19 | K | Joback Method |
| tc | 823.70 | K | Joback Method |
| tf | 402.02 | K | Joback Method |
| vc | 0.711 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 502.19 | J/mol×K | 609.19 | Joback Method |
| cpg | 522.71 | J/mol×K | 644.94 | Joback Method |
| cpg | 542.11 | J/mol×K | 680.69 | Joback Method |
| cpg | 560.36 | J/mol×K | 716.44 | Joback Method |
| cpg | 577.47 | J/mol×K | 752.20 | Joback Method |
| cpg | 593.43 | J/mol×K | 787.95 | Joback Method |
| cpg | 608.23 | J/mol×K | 823.70 | 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=R241079&Units=SI |

# Legend

| | |
|---|---|
| **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 |