

1,3-Hexadiene

| | |
|----------------------|---|
| Inchi: | InChI=1S/C6H10/c1-3-5-6-4-2/h3,5-6H,1,4H2,2H3/b6-5+ |
| InchiKey: | AHAREKHAZNPPMI-AATRIKPKSA-N |
| Formula: | C6H10 |
| SMILES: | C=CC=CCC |
| Mol. weight [g/mol]: | 82.14 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 167.70 | kJ/mol | Joback Method |
| hf | 75.48 | kJ/mol | Joback Method |
| hfus | 10.22 | kJ/mol | Joback Method |
| hvap | 28.24 | kJ/mol | Joback Method |
| log10ws | -2.04 | | Crippen Method |
| logp | 2.139 | | Crippen Method |
| mcvol | 86.800 | ml/mol | McGowan Method |
| pc | 3460.21 | kPa | Joback Method |
| rinpol | 620.00 | | NIST Webbook |
| rinpol | 620.00 | | NIST Webbook |
| tb | 337.52 | K | Joback Method |
| tc | 513.57 | K | Joback Method |
| tf | 150.54 | K | Joback Method |
| vc | 0.333 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 132.12 | J/molxK | 337.52 | Joback Method |
| cpg | 141.86 | J/molxK | 366.86 | Joback Method |
| cpg | 151.13 | J/molxK | 396.20 | Joback Method |
| cpg | 159.96 | J/molxK | 425.54 | Joback Method |
| cpg | 168.36 | J/molxK | 454.89 | Joback Method |
| cpg | 176.34 | J/molxK | 484.23 | Joback Method |
| cpg | 183.93 | J/molxK | 513.57 | Joback Method |
| dvisc | 0.0031761 | Paxs | 150.54 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0012964 | Paxs | 181.70 | Joback Method |
| dvisc | 0.0006879 | Paxs | 212.87 | Joback Method |
| dvisc | 0.0004292 | Paxs | 244.03 | Joback Method |
| dvisc | 0.0002980 | Paxs | 275.19 | Joback Method |
| dvisc | 0.0002228 | Paxs | 306.36 | Joback Method |
| dvisc | 0.0001758 | Paxs | 337.52 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U158236&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/71-939-1/1-3-Hexadiene.pdf>

Generated by Cheméo on 2025-12-22 01:30:08.206727848 +0000 UTC m=+6115205.736768501.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.