

Cyclohexene,1-hexyl-

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|-----------------------------|--|
| Other names: | 1-hexyl-1-cyclohexene |
| Inchi: | InChI=1S/C12H22/c1-2-3-4-6-9-12-10-7-5-8-11-12/h10H,2-9,11H2,1H3 |
| InchiKey: | NEFDOOJYBCQHHV-UHFFFAOYSA-N |
| Formula: | C12H22 |
| SMILES: | CCCCCCC1=CCCCC1 |
| Mol. weight [g/mol]: | 166.30 |
| CAS: | 3964-66-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------------|--------|----------------|
| gf | 102.65 | kJ/mol | Joback Method |
| hf | -170.04 | kJ/mol | Joback Method |
| hfus | 18.43 | kJ/mol | Joback Method |
| hvap | 44.00 | kJ/mol | Joback Method |
| ie | 8.37 ± 0.03 | eV | NIST Webbook |
| log10ws | -4.59 | | Crippen Method |
| logp | 4.457 | | Crippen Method |
| mcvol | 164.780 | ml/mol | McGowan Method |
| pc | 2244.00 | kPa | Joback Method |
| ripol | 1242.00 | | NIST Webbook |
| ripol | 1244.00 | | NIST Webbook |
| ripol | 1243.00 | | NIST Webbook |
| ripol | 1243.00 | | NIST Webbook |
| ripol | 1395.00 | | NIST Webbook |
| ripol | 1414.00 | | NIST Webbook |
| ripol | 1419.00 | | NIST Webbook |
| ripol | 1373.00 | | NIST Webbook |
| ripol | 1379.00 | | NIST Webbook |
| ripol | 1384.00 | | NIST Webbook |
| ripol | 1389.00 | | NIST Webbook |
| ripol | 1403.00 | | NIST Webbook |
| ripol | 1399.00 | | NIST Webbook |
| ripol | 1404.00 | | NIST Webbook |
| ripol | 1373.00 | | NIST Webbook |
| ripol | 1378.60 | | NIST Webbook |
| ripol | 1384.20 | | NIST Webbook |
| ripol | 1389.10 | | NIST Webbook |

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|-------|---------------|---------|---------------|
| ripol | 1394.60 | | NIST Webbook |
| ripol | 1399.20 | | NIST Webbook |
| ripol | 1404.30 | | NIST Webbook |
| ripol | 1388.00 | | NIST Webbook |
| ripol | 1399.00 | | NIST Webbook |
| ripol | 1388.00 | | NIST Webbook |
| ripol | 1354.60 | | NIST Webbook |
| ripol | 1350.00 | | NIST Webbook |
| ripol | 1342.40 | | NIST Webbook |
| tb | 493.00 ± 5.00 | K | NIST Webbook |
| tc | 697.83 | K | Joback Method |
| tf | 249.90 | K | Joback Method |
| vc | 0.627 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 379.55 | J/molxK | 502.32 | Joback Method |
| cpg | 465.80 | J/molxK | 665.24 | Joback Method |
| cpg | 450.33 | J/molxK | 632.66 | Joback Method |
| cpg | 433.99 | J/molxK | 600.07 | Joback Method |
| cpg | 416.77 | J/molxK | 567.49 | Joback Method |
| cpg | 398.64 | J/molxK | 534.90 | Joback Method |
| cpg | 480.45 | J/molxK | 697.83 | Joback Method |
| dvisc | 0.0002099 | Paxs | 502.32 | Joback Method |
| dvisc | 0.0002842 | Paxs | 460.25 | Joback Method |
| dvisc | 0.0004090 | Paxs | 418.18 | Joback Method |
| dvisc | 0.0006385 | Paxs | 376.11 | Joback Method |
| dvisc | 0.0011151 | Paxs | 334.04 | Joback Method |
| dvisc | 0.0022871 | Paxs | 291.97 | Joback Method |
| dvisc | 0.0059743 | Paxs | 249.90 | Joback Method |

Sources

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=C3964667&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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 |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| ripol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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