

Bi-2-cyclohexen-1-yl

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|-----------------------------|---|
| Other names: | 3,3'-Bicyclohexenyl |
| Inchi: | InChI=1S/C12H18/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h3,5,7,9,11-12H,1-2,4,6,8,10H2 |
| InchiKey: | HFROTUORNFKSE-UHFFFAOYSA-N |
| Formula: | C12H18 |
| SMILES: | <chem>C1=CC(C2C=CCCC2)CCC1</chem> |
| Mol. weight [g/mol]: | 162.27 |
| CAS: | 1541-20-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 158.98 | kJ/mol | Joback Method |
| hf | -66.81 | kJ/mol | Joback Method |
| hfus | 12.95 | kJ/mol | Joback Method |
| hvap | 43.75 | kJ/mol | Joback Method |
| log10ws | -3.86 | | Crippen Method |
| logp | 3.699 | | Crippen Method |
| mcvol | 149.620 | ml/mol | McGowan Method |
| pc | 2805.41 | kPa | Joback Method |
| tb | 511.38 | K | Joback Method |
| tc | 748.33 | K | Joback Method |
| tf | 241.28 | K | Joback Method |
| vc | 0.545 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 349.94 | J/molxK | 511.38 | Joback Method |
| cpg | 373.54 | J/molxK | 550.87 | Joback Method |
| cpg | 395.57 | J/molxK | 590.36 | Joback Method |
| cpg | 416.09 | J/molxK | 629.85 | Joback Method |
| cpg | 435.17 | J/molxK | 669.35 | Joback Method |
| cpg | 452.85 | J/molxK | 708.84 | Joback Method |
| cpg | 469.20 | J/molxK | 748.33 | Joback Method |
| dvisc | 0.0067331 | Paxs | 241.28 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0025376 | Paxs | 286.30 | Joback Method |
| dvisc | 0.0012468 | Paxs | 331.31 | Joback Method |
| dvisc | 0.0007261 | Paxs | 376.33 | Joback Method |
| dvisc | 0.0004747 | Paxs | 421.35 | Joback Method |
| dvisc | 0.0003368 | Paxs | 466.36 | Joback Method |
| dvisc | 0.0002539 | Paxs | 511.38 | 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=C1541204&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|---|
| cp_g: | 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: | Log ₁₀ 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 |

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