

Cyclohexene, 3-iodo

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|-----------------------------|---|
| Inchi: | InChI=1S/C6H9I/c7-6-4-2-1-3-5-6/h2,4,6H,1,3,5H2 |
| InchiKey: | HQZFWVYLQAPSHX-UHFFFAOYSA-N |
| Formula: | C6H9I |
| SMILES: | IC1C=CCCC1 |
| Mol. weight [g/mol]: | 208.04 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 112.17 | kJ/mol | Joback Method |
| hf | 21.80 | kJ/mol | Joback Method |
| hfus | 8.76 | kJ/mol | Joback Method |
| hvap | 39.04 | kJ/mol | Joback Method |
| log10ws | -3.14 | | Crippen Method |
| logp | 2.530 | | Crippen Method |
| mcvol | 106.060 | ml/mol | McGowan Method |
| pc | 4031.24 | kPa | Joback Method |
| rinpol | 1075.00 | | NIST Webbook |
| rinpol | 1075.00 | | NIST Webbook |
| tb | 448.53 | K | Joback Method |
| tc | 697.74 | K | Joback Method |
| tf | 223.58 | K | Joback Method |
| vc | 0.379 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 175.10 | J/molxK | 448.53 | Joback Method |
| cpg | 188.79 | J/molxK | 490.06 | Joback Method |
| cpg | 201.50 | J/molxK | 531.60 | Joback Method |
| cpg | 213.28 | J/molxK | 573.13 | Joback Method |
| cpg | 224.17 | J/molxK | 614.67 | Joback Method |
| cpg | 234.23 | J/molxK | 656.20 | Joback Method |
| cpg | 243.50 | J/molxK | 697.74 | Joback Method |
| dvisc | 0.0067198 | Paxs | 223.58 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0029927 | Paxs | 261.07 | Joback Method |
| dvisc | 0.0016331 | Paxs | 298.56 | Joback Method |
| dvisc | 0.0010201 | Paxs | 336.05 | Joback Method |
| dvisc | 0.0007003 | Paxs | 373.55 | Joback Method |
| dvisc | 0.0005149 | Paxs | 411.04 | Joback Method |
| dvisc | 0.0003986 | Paxs | 448.53 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=R25455&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |

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<https://www.chemeo.com/cid/62-075-0/Cyclohexene-3-iodo.pdf>

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