

Cyclohexene, 4-iodo-5-methyl

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| Inchi: | InChI=1S/C7H11I/c1-6-4-2-3-5-7(6)8/h2-3,6-7H,4-5H2,1H3 |
| InchiKey: | ZLSMUALXYOVSQT-UHFFFAOYSA-N |
| Formula: | C7H11I |
| SMILES: | CC1CC=CCC1I |
| Mol. weight [g/mol]: | 222.07 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 112.88 | kJ/mol | Joback Method |
| hf | -19.18 | kJ/mol | Joback Method |
| hfus | 12.42 | kJ/mol | Joback Method |
| hvap | 40.96 | kJ/mol | Joback Method |
| log10ws | -3.32 | | Crippen Method |
| logp | 2.776 | | Crippen Method |
| mcvol | 120.150 | ml/mol | McGowan Method |
| pc | 3443.98 | kPa | Joback Method |
| rinsol | 1152.00 | | NIST Webbook |
| tb | 466.74 | K | Joback Method |
| tc | 711.31 | K | Joback Method |
| tf | 230.61 | K | Joback Method |
| vc | 0.433 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 216.79 | J/molxK | 466.74 | Joback Method |
| cpg | 232.17 | J/molxK | 507.50 | Joback Method |
| cpg | 246.55 | J/molxK | 548.26 | Joback Method |
| cpg | 259.95 | J/molxK | 589.03 | Joback Method |
| cpg | 272.43 | J/molxK | 629.79 | Joback Method |
| cpg | 284.03 | J/molxK | 670.55 | Joback Method |
| cpg | 294.77 | J/molxK | 711.31 | Joback Method |
| dvisc | 0.0043183 | Paxs | 230.61 | Joback Method |
| dvisc | 0.0021465 | Paxs | 269.97 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0012747 | Paxs | 309.32 | Joback Method |
| dvisc | 0.0008514 | Paxs | 348.68 | Joback Method |
| dvisc | 0.0006173 | Paxs | 388.03 | Joback Method |
| dvisc | 0.0004748 | Paxs | 427.38 | Joback Method |
| dvisc | 0.0003817 | Paxs | 466.74 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R25491&Units=SI |

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/32-995-2/Cyclohexene-4-iodo-5-methyl.pdf>

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