

Hexane, 2,3-dichloro-, erythro

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|-----------------------------|---|
| Other names: | 2,3-dichlorohexane (erythro) |
| Inchi: | InChI=1S/C6H12Cl2/c1-3-4-6(8)5(2)7/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1 |
| InchiKey: | IILOKMKZRPIYGG-WDSKDSINSA-N |
| Formula: | C6H12Cl2 |
| SMILES: | CCCC(CI)C(C)CI |
| Mol. weight [g/mol]: | 155.06 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -29.10 | kJ/mol | Joback Method |
| hf | -209.21 | kJ/mol | Joback Method |
| hfus | 12.64 | kJ/mol | Joback Method |
| hvap | 36.94 | kJ/mol | Joback Method |
| log10ws | -2.86 | | Crippen Method |
| logp | 3.021 | | Crippen Method |
| mcvol | 119.880 | ml/mol | McGowan Method |
| pc | 2915.53 | kPa | Joback Method |
| rinpol | 965.00 | | NIST Webbook |
| ripol | 1231.00 | | NIST Webbook |
| ripol | 1231.00 | | NIST Webbook |
| tb | 410.66 | K | Joback Method |
| tc | 599.28 | K | Joback Method |
| tf | 187.22 | K | Joback Method |
| vc | 0.458 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 212.29 | J/molxK | 410.66 | Joback Method |
| cpg | 223.08 | J/molxK | 442.10 | Joback Method |
| cpg | 233.37 | J/molxK | 473.53 | Joback Method |
| cpg | 243.19 | J/molxK | 504.97 | Joback Method |
| cpg | 252.55 | J/molxK | 536.41 | Joback Method |
| cpg | 261.47 | J/molxK | 567.84 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 269.95 | J/mol×K | 599.28 | Joback Method |
| dvisc | 0.0130601 | Paxs | 187.22 | Joback Method |
| dvisc | 0.0041501 | Paxs | 224.46 | Joback Method |
| dvisc | 0.0018276 | Paxs | 261.70 | Joback Method |
| dvisc | 0.0009873 | Paxs | 298.94 | Joback Method |
| dvisc | 0.0006113 | Paxs | 336.18 | Joback Method |
| dvisc | 0.0004165 | Paxs | 373.42 | Joback Method |
| dvisc | 0.0003042 | Paxs | 410.66 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R211840&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

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|------------------|---|
| 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 |
| rinpolar: | Non-polar retention indices |
| ripolar: | 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/37-372-8/Hexane-2-3-dichloro-erythro.pdf>

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