

5-Ethylindan

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|-----------------------------|---|
| Inchi: | InChI=1S/C11H14/c1-2-9-6-7-10-4-3-5-11(10)8-9/h6-8H,2-5H2,1H3 |
| InchiKey: | IFKCGHPIWWIUOG-UHFFFAOYSA-N |
| Formula: | C11H14 |
| SMILES: | CCc1ccc2c(c1)CCC2 |
| Mol. weight [g/mol]: | 146.23 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 203.35 | kJ/mol | Joback Method |
| hf | 36.36 | kJ/mol | Joback Method |
| hfus | 14.57 | kJ/mol | Joback Method |
| hvap | 43.90 | kJ/mol | Joback Method |
| log10ws | -3.36 | | Crippen Method |
| logp | 2.738 | | Crippen Method |
| mcvol | 131.230 | ml/mol | McGowan Method |
| pc | 3052.41 | kPa | Joback Method |
| rinpol | 1243.34 | | NIST Webbook |
| rinpol | 1238.62 | | NIST Webbook |
| rinpol | 1231.25 | | NIST Webbook |
| rinpol | 1217.04 | | NIST Webbook |
| rinpol | 1212.73 | | NIST Webbook |
| rinpol | 1206.07 | | NIST Webbook |
| tb | 499.13 | K | Joback Method |
| tc | 720.35 | K | Joback Method |
| tf | 287.37 | K | Joback Method |
| vc | 0.501 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 286.20 | J/molxK | 499.13 | Joback Method |
| cpg | 302.20 | J/molxK | 536.00 | Joback Method |
| cpg | 317.14 | J/molxK | 572.87 | Joback Method |
| cpg | 331.10 | J/molxK | 609.74 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 344.13 | J/molxK | 646.61 | Joback Method |
| cpg | 356.30 | J/molxK | 683.48 | Joback Method |
| cpg | 367.68 | J/molxK | 720.35 | Joback Method |
| dvisc | 0.0016819 | Paxs | 287.37 | Joback Method |
| dvisc | 0.0011456 | Paxs | 322.66 | Joback Method |
| dvisc | 0.0008416 | Paxs | 357.96 | Joback Method |
| dvisc | 0.0006535 | Paxs | 393.25 | Joback Method |
| dvisc | 0.0005290 | Paxs | 428.54 | Joback Method |
| dvisc | 0.0004423 | Paxs | 463.84 | Joback Method |
| dvisc | 0.0003792 | Paxs | 499.13 | 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=R250647&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 |
| 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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