

Cyclohexane, 1r,2c,4c-tris-ethenyl

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H18/c1-4-10-7-8-11(5-2)12(6-3)9-10/h4-6,10-12H,1-3,7-9H2/t10-,11+,12-/m |
| InchiKey: | KTRQRAQRHBLCSQ-TUAOUCFPSA-N |
| Formula: | C12H18 |
| SMILES: | C=CC1CCC(C=C)C(C=C)C1 |
| Mol. weight [g/mol]: | 162.27 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 322.71 | kJ/mol | Joback Method |
| hf | 98.92 | kJ/mol | Joback Method |
| hfus | 16.97 | kJ/mol | Joback Method |
| hvap | 40.11 | kJ/mol | Joback Method |
| log10ws | -3.58 | | Crippen Method |
| logp | 3.577 | | Crippen Method |
| mcvol | 156.180 | ml/mol | McGowan Method |
| pc | 2256.81 | kPa | Joback Method |
| rinpol | 1114.00 | | NIST Webbook |
| tb | 474.21 | K | Joback Method |
| tc | 678.46 | K | Joback Method |
| tf | 218.62 | K | Joback Method |
| vc | 0.582 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 340.41 | J/molxK | 474.21 | Joback Method |
| cpg | 431.53 | J/molxK | 644.42 | Joback Method |
| cpg | 415.30 | J/molxK | 610.38 | Joback Method |
| cpg | 398.11 | J/molxK | 576.33 | Joback Method |
| cpg | 379.92 | J/molxK | 542.29 | Joback Method |
| cpg | 360.70 | J/molxK | 508.25 | Joback Method |
| cpg | 446.82 | J/molxK | 678.46 | Joback Method |
| dvisc | 0.0002602 | Paxs | 474.21 | Joback Method |
| dvisc | 0.0003121 | Paxs | 431.61 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003895 | Paxs | 389.01 | Joback Method |
| dvisc | 0.0005134 | Paxs | 346.41 | Joback Method |
| dvisc | 0.0007313 | Paxs | 303.82 | Joback Method |
| dvisc | 0.0011689 | Paxs | 261.22 | Joback Method |
| dvisc | 0.0022430 | Paxs | 218.62 | 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=R10892&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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/36-273-9/Cyclohexane-1r-2c-4c-tris-ethenyl.pdf>

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