

3-Cyclohexene-1-ethanol, «alpha»-ethenyl-«alpha»,3-dimethyl-6-(1-methylet

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|-----------------------------|-----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C15H24O/c1-6-15(5,16)10-13-9-12(4)7-8-14(13)11(2)3/h6-7,13,16H,1,8-10H2, |
| InchiKey: | LCXFGBNEANUFOH-UHFFFAOYSA-N |
| Formula: | C15H24O |
| SMILES: | C=CC(C)(O)CC1CC(C)=CCC1=C(C)C |
| Mol. weight [g/mol]: | 220.35 |
| CAS: | 55780-93-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 110.97 | kJ/mol | Joback Method |
| hf | -221.61 | kJ/mol | Joback Method |
| hfus | 21.68 | kJ/mol | Joback Method |
| hvap | 65.95 | kJ/mol | Joback Method |
| log10ws | -4.69 | | Crippen Method |
| logp | 4.006 | | Crippen Method |
| mcvol | 204.320 | ml/mol | McGowan Method |
| pc | 1984.12 | kPa | Joback Method |
| tb | 658.44 | K | Joback Method |
| tc | 857.63 | K | Joback Method |
| tf | 337.35 | K | Joback Method |
| vc | 0.767 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 565.82 | J/molxK | 658.44 | Joback Method |
| cpg | 582.91 | J/molxK | 691.64 | Joback Method |
| cpg | 599.00 | J/molxK | 724.84 | Joback Method |
| cpg | 614.14 | J/molxK | 758.03 | Joback Method |
| cpg | 628.40 | J/molxK | 791.23 | Joback Method |
| cpg | 641.83 | J/molxK | 824.43 | Joback Method |
| cpg | 654.48 | J/molxK | 857.63 | 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=C55780933&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|-------------------------------------------------|
| cpg: | Ideal gas heat capacity |
| 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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