

1,1-Bis(ethylcyclohexyl)ethane

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|-----------------------------|---|
| Inchi: | InChI=1S/C18H34/c1-4-17(12-8-6-9-13-17)16(3)18(5-2)14-10-7-11-15-18/h16H,4-15H2,1 |
| InchiKey: | HXBDGYWGALHERR-UHFFFAOYSA-N |
| Formula: | C18H34 |
| SMILES: | CCC1(C(C)C2(CC)CCCCC2)CCCCC1 |
| Mol. weight [g/mol]: | 250.46 |
| CAS: | 98803-07-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 136.16 | kJ/mol | Joback Method |
| hf | -281.01 | kJ/mol | Joback Method |
| hfus | 9.93 | kJ/mol | Joback Method |
| hvap | 53.83 | kJ/mol | Joback Method |
| log10ws | -6.42 | | Crippen Method |
| logp | 6.344 | | Crippen Method |
| mcvol | 242.760 | ml/mol | McGowan Method |
| pc | 1682.41 | kPa | Joback Method |
| tb | 650.38 | K | Joback Method |
| tc | 879.20 | K | Joback Method |
| tf | 340.18 | K | Joback Method |
| vc | 0.899 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 836.77 | J/molxK | 841.06 | Joback Method |
| cpg | 711.04 | J/molxK | 650.38 | Joback Method |
| cpg | 738.53 | J/molxK | 688.52 | Joback Method |
| cpg | 764.58 | J/molxK | 726.65 | Joback Method |
| cpg | 789.45 | J/molxK | 764.79 | Joback Method |
| cpg | 813.42 | J/molxK | 802.92 | Joback Method |
| cpg | 859.75 | J/molxK | 879.20 | Joback Method |
| cpl | 477.80 | J/molxK | 313.00 | NIST Webbook |

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=C98803077&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 |
| cpl: | Liquid phase 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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