

(E,E,Z)-Bicyclo[10.1.0]trideca-4,8-diene

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|----------------------|--|
| Inchi: | InChI=1S/C13H20/c1-2-4-6-8-10-13-11-12(13)9-7-5-3-1/h3-6,12-13H,1-2,7-11H2/b5-3+,6 |
| InchiKey: | OKQPAVLKCLUCOF-JKODOUFDSA-N |
| Formula: | C13H20 |
| SMILES: | C1=CCCC2CC2CCC=CCC1 |
| Mol. weight [g/mol]: | 176.30 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 155.30 | kJ/mol | Joback Method |
| hf | -93.61 | kJ/mol | Joback Method |
| hfus | 13.44 | kJ/mol | Joback Method |
| hvap | 46.15 | kJ/mol | Joback Method |
| log10ws | -4.28 | | Crippen Method |
| logp | 4.089 | | Crippen Method |
| mcvol | 163.710 | ml/mol | McGowan Method |
| pc | 2605.74 | kPa | Joback Method |
| rinsol | 1372.00 | | NIST Webbook |
| tb | 538.53 | K | Joback Method |
| tc | 779.84 | K | Joback Method |
| tf | 249.03 | K | Joback Method |
| vc | 0.594 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 401.16 | J/molxK | 538.53 | Joback Method |
| cpg | 511.18 | J/molxK | 739.62 | Joback Method |
| cpg | 492.38 | J/molxK | 699.40 | Joback Method |
| cpg | 472.03 | J/molxK | 659.18 | Joback Method |
| cpg | 450.08 | J/molxK | 618.97 | Joback Method |
| cpg | 426.48 | J/molxK | 578.75 | Joback Method |
| cpg | 528.50 | J/molxK | 779.84 | Joback Method |
| dvisc | 0.0001897 | Paxs | 538.53 | Joback Method |
| dvisc | 0.0002638 | Paxs | 490.28 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003942 | Paxs | 442.03 | Joback Method |
| dvisc | 0.0006502 | Paxs | 393.78 | Joback Method |
| dvisc | 0.0012331 | Paxs | 345.53 | Joback Method |
| dvisc | 0.0028788 | Paxs | 297.28 | Joback Method |
| dvisc | 0.0093345 | Paxs | 249.03 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R2809&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

| | |
|-----------------|---|
| 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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<https://www.chemeo.com/cid/70-755-6/E-E-Z-Bicyclo-10-1-0-trideca-4-8-diene.pdf>

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