

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

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|-----------------------------|---|
| Inchi: | InChI=1S/C15H24/c1-14-11-9-7-5-3-4-6-8-10-12-15(14,2)13-14/h5-8H,3-4,9-13H2,1-2H3 |
| InchiKey: | PFXKPLMGASGUIW-DVJYWQQMSA-N |
| Formula: | C15H24 |
| SMILES: | CC12CCC=CCCC=CCCC1(C)C2 |
| Mol. weight [g/mol]: | 204.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 161.16 | kJ/mol | Joback Method |
| hf | -104.41 | kJ/mol | Joback Method |
| hfus | 6.02 | kJ/mol | Joback Method |
| hvap | 48.30 | kJ/mol | Joback Method |
| log10ws | -5.11 | | Crippen Method |
| logp | 4.869 | | Crippen Method |
| mcvol | 191.890 | ml/mol | McGowan Method |
| pc | 2354.20 | kPa | Joback Method |
| rinpol | 1405.00 | | NIST Webbook |
| rinpol | 1405.00 | | NIST Webbook |
| tb | 584.77 | K | Joback Method |
| tc | 836.47 | K | Joback Method |
| tf | 319.37 | K | Joback Method |
| vc | 0.702 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 503.32 | J/molxK | 584.77 | Joback Method |
| cpg | 529.07 | J/molxK | 626.72 | Joback Method |
| cpg | 553.00 | J/molxK | 668.67 | Joback Method |
| cpg | 575.45 | J/molxK | 710.62 | Joback Method |
| cpg | 596.75 | J/molxK | 752.57 | Joback Method |
| cpg | 617.25 | J/molxK | 794.52 | Joback Method |
| cpg | 637.28 | J/molxK | 836.47 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R3020&Units=SI |

Legend

| | |
|----------------------------|---|
| cp_g: | Ideal gas heat capacity |
| g_f: | Standard Gibbs free energy of formation |
| h_f: | Enthalpy of formation at standard conditions |
| h_{fus}: | Enthalpy of fusion at standard conditions |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mc_{vol}: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rin_{pol}: | 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/14-277-9/Z-E-Z-Bicyclo-10-1-0-trideca-4-8-diene.pdf>

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