

trans-3-Caren-2-ol

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|-----------------------------|--|
| Inchi: | InChI=1S/C10H16O/c1-6-4-5-7-8(9(6)11)10(7,2)3/h4,7-9,11H,5H2,1-3H3 |
| InchiKey: | YCAQPZXDWPYBD-UHFFFAOYSA-N |
| Formula: | C10H16O |
| SMILES: | CC1=CCC2C(C1O)C2(C)C |
| Mol. weight [g/mol]: | 152.23 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 5.32 | kJ/mol | Joback Method |
| hf | -241.65 | kJ/mol | Joback Method |
| hfus | 16.59 | kJ/mol | Joback Method |
| hvap | 53.72 | kJ/mol | Joback Method |
| log10ws | -2.30 | | Crippen Method |
| logp | 1.969 | | Crippen Method |
| mcvol | 131.610 | ml/mol | McGowan Method |
| pc | 3082.99 | kPa | Joback Method |
| ripol | 1727.00 | | NIST Webbook |
| tb | 533.17 | K | Joback Method |
| tc | 729.30 | K | Joback Method |
| tf | 324.34 | K | Joback Method |
| vc | 0.502 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 336.85 | J/mol×K | 533.17 | Joback Method |
| cpg | 351.53 | J/mol×K | 565.86 | Joback Method |
| cpg | 365.30 | J/mol×K | 598.55 | Joback Method |
| cpg | 378.26 | J/mol×K | 631.23 | Joback Method |
| cpg | 390.53 | J/mol×K | 663.92 | Joback Method |
| cpg | 402.21 | J/mol×K | 696.61 | Joback Method |
| cpg | 413.40 | J/mol×K | 729.30 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U151754&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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|---|
| 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 |
| riPOL: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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