

Thujen-3-en-10-ol

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C10H16O/c1-7(2)10-4-3-8(6-11)9(10)5-10/h3,7,9,11H,4-6H2,1-2H3 |
| InchiKey: | NWXGYXZDAFRGSL-UHFFFAOYSA-N |
| Formula: | C10H16O |
| SMILES: | CC(C)C12CC=C(CO)C1C2 |
| Mol. weight [g/mol]: | 152.23 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 30.40 | kJ/mol | Joback Method |
| hf | -200.09 | kJ/mol | Joback Method |
| hfus | 13.03 | kJ/mol | Joback Method |
| hvap | 53.77 | kJ/mol | Joback Method |
| log10ws | -2.19 | | Crippen Method |
| logp | 1.971 | | Crippen Method |
| mcvol | 131.610 | ml/mol | McGowan Method |
| pc | 3257.86 | kPa | Joback Method |
| rinpol | 1184.00 | | NIST Webbook |
| tb | 537.80 | K | Joback Method |
| tc | 731.69 | K | Joback Method |
| tf | 321.34 | K | Joback Method |
| vc | 0.506 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 334.33 | J/mol×K | 537.80 | Joback Method |
| cpg | 347.74 | J/mol×K | 570.12 | Joback Method |
| cpg | 360.24 | J/mol×K | 602.43 | Joback Method |
| cpg | 371.96 | J/mol×K | 634.75 | Joback Method |
| cpg | 383.01 | J/mol×K | 667.06 | Joback Method |
| cpg | 393.52 | J/mol×K | 699.38 | Joback Method |
| cpg | 403.61 | J/mol×K | 731.69 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R516848&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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/55-570-8/Thujen-3-en-10-ol.pdf>

Generated by Cheméo on 2024-04-27 22:13:40.848301693 +0000 UTC m=+16545269.768879008.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.