

Bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)-

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|----------------------|--|
| Other names: | 3-Thujanone Chrysanthone Tanacetone 1-Isopropyl-4-methylbicyclo[3.1.0]hexan-3-one (-)-Thujone Thujan-3-one NSC 407281 Thujone |
| Inchi: | InChI=1S/C10H16O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-8H,4-5H2,1-3H3 |
| InchiKey: | USMNOWBWPHYOEAE-UHFFFAOYSA-N |
| Formula: | C10H16O |
| SMILES: | CC1C(=O)CC2(C(C)C)CC12 |
| Mol. weight [g/mol]: | 152.23 |
| CAS: | 1125-12-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| chl | -5991.10 | kJ/mol | NIST Webbook |
| gf | 16.59 | kJ/mol | Joback Method |
| hf | -252.21 | kJ/mol | Joback Method |
| hfus | 8.69 | kJ/mol | Joback Method |
| hvap | 40.08 | kJ/mol | Joback Method |
| log10ws | -2.11 | | Crippen Method |
| logp | 2.258 | | Crippen Method |
| mcvol | 131.610 | ml/mol | McGowan Method |
| pc | 2881.21 | kPa | Joback Method |
| rinpol | 1114.00 | | NIST Webbook |
| rinpol | 1114.00 | | NIST Webbook |
| rinpol | 1124.00 | | NIST Webbook |
| tb | 358.20 | K | NIST Webbook |
| tc | 724.49 | K | Joback Method |
| tf | 311.22 | K | Joback Method |
| vc | 0.507 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 324.27 | J/mol×K | 504.63 | Joback Method |
| cpg | 342.10 | J/mol×K | 541.27 | Joback Method |
| cpg | 358.73 | J/mol×K | 577.92 | Joback Method |
| cpg | 374.30 | J/mol×K | 614.56 | Joback Method |
| cpg | 388.94 | J/mol×K | 651.20 | Joback Method |
| cpg | 402.80 | J/mol×K | 687.84 | Joback Method |
| cpg | 416.01 | J/mol×K | 724.49 | 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=C1125128&Units=SI |

Legend

| | |
|-----------------|---|
| chl: | Standard liquid enthalpy of combustion |
| 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 |

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