

Tetrahydrofuran, 3-isopropyl-2-(3-methylcyclopent-2-enyl)

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| Inchi: | InChI=1S/C13H22O/c1-9(2)11-7-8-14-13(11)12-6-4-5-10(12)3/h6,9-11,13H,4-5,7-8H2,1-3 |
| InchiKey: | RLVBOJOICUKZPB-UHFFFAOYSA-N |
| Formula: | C13H22O |
| SMILES: | CC1CCC=C1C1OCCC1C(C)C |
| Mol. weight [g/mol]: | 194.31 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 55.74 | kJ/mol | Joback Method |
| hf | -302.00 | kJ/mol | Joback Method |
| hfus | 23.66 | kJ/mol | Joback Method |
| hvap | 49.81 | kJ/mol | Joback Method |
| log10ws | -3.38 | | Crippen Method |
| logp | 3.404 | | Crippen Method |
| mcvol | 173.880 | ml/mol | McGowan Method |
| pc | 2227.09 | kPa | Joback Method |
| rinpol | 1390.00 | | NIST Webbook |
| rinpol | 1390.00 | | NIST Webbook |
| ripol | 1705.00 | | NIST Webbook |
| ripol | 1705.00 | | NIST Webbook |
| tb | 553.38 | K | Joback Method |
| tc | 771.11 | K | Joback Method |
| tf | 278.68 | K | Joback Method |
| vc | 0.645 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 453.33 | J/molxK | 553.38 | Joback Method |
| cpg | 475.78 | J/molxK | 589.67 | Joback Method |
| cpg | 496.90 | J/molxK | 625.96 | Joback Method |
| cpg | 516.76 | J/molxK | 662.24 | Joback Method |
| cpg | 535.39 | J/molxK | 698.53 | Joback Method |
| cpg | 552.83 | J/molxK | 734.82 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 569.15 | J/molxK | 771.11 | Joback Method |
| dvisc | 0.0033995 | Paxs | 278.68 | Joback Method |
| dvisc | 0.0018271 | Paxs | 324.46 | Joback Method |
| dvisc | 0.0011450 | Paxs | 370.25 | Joback Method |
| dvisc | 0.0007952 | Paxs | 416.03 | Joback Method |
| dvisc | 0.0005937 | Paxs | 461.81 | Joback Method |
| dvisc | 0.0004673 | Paxs | 507.60 | Joback Method |
| dvisc | 0.0003826 | Paxs | 553.38 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=R199309&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| ripol: | Non-polar retention indices |
| ripol: | 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/80-064-2/Tetrahydrofuran-3-isopropyl-2-3-methylcyclopent-2-enyl.pdf>

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