

1-trans-3-methylisopropylcyclopentane

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|-----------------------------|--|
| Other names: | trans-1-Methyl-3-isopropylcyclopentane Cyclopentane, 1-methyl-3-(1-methylethyl)-, trans |
| Inchi: | InChI=1S/C9H18/c1-7(2)9-5-4-8(3)6-9/h7-9H,4-6H2,1-3H3/t8-,9-/m1/s1 |
| InchiKey: | CDTDMKCVKCGRPD-RKDXNWHRSA-N |
| Formula: | C9H18 |
| SMILES: | CC1CCC(C(C)C)C1 |
| Mol. weight [g/mol]: | 126.24 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 51.30 | kJ/mol | Joback Method |
| hf | -194.23 | kJ/mol | Joback Method |
| hfus | 10.55 | kJ/mol | Joback Method |
| hvap | 35.19 | kJ/mol | Joback Method |
| log10ws | -2.76 | | Crippen Method |
| logp | 3.079 | | Crippen Method |
| mcvol | 126.810 | ml/mol | McGowan Method |
| pc | 2693.00 | kPa | Joback Method |
| rinpol | 865.00 | | NIST Webbook |
| rinpol | 867.00 | | NIST Webbook |
| rinpol | 869.00 | | NIST Webbook |
| rinpol | 856.00 | | NIST Webbook |
| rinpol | 859.60 | | NIST Webbook |
| rinpol | 862.00 | | NIST Webbook |
| rinpol | 872.00 | | NIST Webbook |
| rinpol | 862.00 | | NIST Webbook |
| tb | 415.49 | K | Joback Method |
| tc | 610.70 | K | Joback Method |
| tf | 182.85 | K | Joback Method |
| vc | 0.473 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
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|-------|-----------|---------|--------|---------------|
| cpg | 255.75 | J/molxK | 415.49 | Joback Method |
| cpg | 339.06 | J/molxK | 578.17 | Joback Method |
| cpg | 323.99 | J/molxK | 545.63 | Joback Method |
| cpg | 308.15 | J/molxK | 513.10 | Joback Method |
| cpg | 291.51 | J/molxK | 480.56 | Joback Method |
| cpg | 274.05 | J/molxK | 448.03 | Joback Method |
| cpg | 353.37 | J/molxK | 610.70 | Joback Method |
| dvisc | 0.0002863 | Paxs | 415.49 | Joback Method |
| dvisc | 0.0003541 | Paxs | 376.72 | Joback Method |
| dvisc | 0.0004600 | Paxs | 337.94 | Joback Method |
| dvisc | 0.0006395 | Paxs | 299.17 | Joback Method |
| dvisc | 0.0009806 | Paxs | 260.40 | Joback Method |
| dvisc | 0.0017463 | Paxs | 221.62 | Joback Method |
| dvisc | 0.0039722 | Paxs | 182.85 | 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=R93038&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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

tf: Normal melting (fusion) point

vc: Critical Volume

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