

(3aRS,4SR,7aRS)-(Octahydro-1H-inden-4-yl) methanol

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| Inchi: | InChI=1S/C10H18O/c11-7-9-5-1-3-8-4-2-6-10(8)9/h8-11H,1-7H2 |
| InchiKey: | JAZXFQSTFJATMJ-UHFFFAOYSA-N |
| Formula: | C10H18O |
| SMILES: | OCC1CCCC2CCCC12 |
| Mol. weight [g/mol]: | 154.25 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -26.01 | kJ/mol | Joback Method |
| hf | -295.18 | kJ/mol | Joback Method |
| hfus | 16.79 | kJ/mol | Joback Method |
| hvap | 54.57 | kJ/mol | Joback Method |
| log10ws | -2.34 | | Crippen Method |
| logp | 2.195 | | Crippen Method |
| mcvol | 135.910 | ml/mol | McGowan Method |
| pc | 3142.03 | kPa | Joback Method |
| rinpol | 1316.00 | | NIST Webbook |
| rinpol | 1316.00 | | NIST Webbook |
| ripol | 2006.00 | | NIST Webbook |
| tb | 542.00 | K | Joback Method |
| tc | 741.43 | K | Joback Method |
| tf | 284.36 | K | Joback Method |
| vc | 0.503 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 355.79 | J/molxK | 542.00 | Joback Method |
| cpg | 373.42 | J/molxK | 575.24 | Joback Method |
| cpg | 390.04 | J/molxK | 608.48 | Joback Method |
| cpg | 405.70 | J/molxK | 641.72 | Joback Method |
| cpg | 420.44 | J/molxK | 674.96 | Joback Method |
| cpg | 434.31 | J/molxK | 708.20 | Joback Method |
| cpg | 447.36 | J/molxK | 741.43 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0142324 | Paxs | 284.36 | Joback Method |
| dvisc | 0.0048522 | Paxs | 327.30 | Joback Method |
| dvisc | 0.0021233 | Paxs | 370.24 | Joback Method |
| dvisc | 0.0011033 | Paxs | 413.18 | Joback Method |
| dvisc | 0.0006485 | Paxs | 456.12 | Joback Method |
| dvisc | 0.0004176 | Paxs | 499.06 | Joback Method |
| dvisc | 0.0002884 | Paxs | 542.00 | 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=R586684&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 |
| mvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | 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/76-682-1/3aRS-4SR-7aRS-Octahydro-1H-inden-4-yl-methanol.pdf>

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