

4,5-dimethyloctane, racemic

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|-----------------------------|------------------------------------------------------------------------|
| Other names: | 4,5-Dimethyloctane, threo |
| Inchi: | InChI=1S/C10H22/c1-5-7-9(3)10(4)8-6-2/h9-10H,5-8H2,1-4H3/t9-,10-/m0/s1 |
| InchiKey: | DOYJTLUPPPUSMD-UWVGGRQHSA-N |
| Formula: | C10H22 |
| SMILES: | CCCC(C)C(C)CCC |
| Mol. weight [g/mol]: | 142.28 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 28.44 | kJ/mol | Joback Method |
| hf | -260.29 | kJ/mol | Joback Method |
| hfus | 14.61 | kJ/mol | Joback Method |
| hvap | 37.08 | kJ/mol | Joback Method |
| log10ws | -3.52 | | Crippen Method |
| logp | 3.859 | | Crippen Method |
| mcvol | 151.760 | ml/mol | McGowan Method |
| pc | 2139.38 | kPa | Joback Method |
| rinpol | 946.50 | | NIST Webbook |
| rinpol | 942.80 | | NIST Webbook |
| rinpol | 942.80 | | NIST Webbook |
| tb | 427.32 | K | Joback Method |
| tc | 596.92 | K | Joback Method |
| tf | 172.46 | K | Joback Method |
| vc | 0.584 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 315.26 | J/molxK | 427.32 | Joback Method |
| cpg | 388.93 | J/molxK | 568.65 | Joback Method |
| cpg | 375.35 | J/molxK | 540.39 | Joback Method |
| cpg | 361.21 | J/molxK | 512.12 | Joback Method |
| cpg | 346.50 | J/molxK | 483.85 | Joback Method |
| cpg | 331.18 | J/molxK | 455.59 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 401.95 | J/mol×K | 596.92 | Joback Method |
| dvisc | 0.0002171 | Paxs | 427.32 | Joback Method |
| dvisc | 0.0003059 | Paxs | 384.84 | Joback Method |
| dvisc | 0.0004693 | Paxs | 342.37 | Joback Method |
| dvisc | 0.0008129 | Paxs | 299.89 | Joback Method |
| dvisc | 0.0016877 | Paxs | 257.41 | Joback Method |
| dvisc | 0.0046771 | Paxs | 214.94 | Joback Method |
| dvisc | 0.0214146 | Paxs | 172.46 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R293471&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 |

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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