

Octane, 6-ethyl-2-methyl-

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|-----------------------------|--|
| Inchi: | InChI=1S/C11H24/c1-5-11(6-2)9-7-8-10(3)4/h10-11H,5-9H2,1-4H3 |
| InchiKey: | AZXGABNJUBNOHW-UHFFFAOYSA-N |
| Formula: | C11H24 |
| SMILES: | CCC(CC)CCCC(C)C |
| Mol. weight [g/mol]: | 156.31 |
| CAS: | 62016-19-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 36.86 | kJ/mol | Joback Method |
| hf | -280.93 | kJ/mol | Joback Method |
| hfus | 17.20 | kJ/mol | Joback Method |
| hvap | 39.30 | kJ/mol | Joback Method |
| log10ws | -3.94 | | Crippen Method |
| logp | 4.249 | | Crippen Method |
| mcvol | 165.850 | ml/mol | McGowan Method |
| pc | 1961.34 | kPa | Joback Method |
| tb | 450.20 | K | Joback Method |
| tc | 618.81 | K | Joback Method |
| tf | 183.73 | K | Joback Method |
| vc | 0.639 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 360.12 | J/molxK | 450.20 | Joback Method |
| cpg | 437.81 | J/molxK | 590.71 | Joback Method |
| cpg | 423.51 | J/molxK | 562.61 | Joback Method |
| cpg | 408.60 | J/molxK | 534.51 | Joback Method |
| cpg | 393.08 | J/molxK | 506.40 | Joback Method |
| cpg | 376.92 | J/molxK | 478.30 | Joback Method |
| cpg | 451.53 | J/molxK | 618.81 | Joback Method |
| dvisc | 0.0002057 | Paxs | 450.20 | Joback Method |
| dvisc | 0.0002907 | Paxs | 405.79 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0004471 | Paxs | 361.38 | Joback Method |
| dvisc | 0.0007760 | Paxs | 316.96 | Joback Method |
| dvisc | 0.0016118 | Paxs | 272.55 | Joback Method |
| dvisc | 0.0044499 | Paxs | 228.14 | Joback Method |
| dvisc | 0.0200727 | Paxs | 183.73 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C62016197&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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