

Zizanene

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|-----------------------------|---|
| Inchi: | InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h6,9-10,13-15H,5,7-8H2 |
| InchiKey: | QMAYBMKBYCGXDH-WLYUNCDWSA-N |
| Formula: | C15H24 |
| SMILES: | CC1=CC2C(CC1)C(C)=CCC2C(C)C |
| Mol. weight [g/mol]: | 204.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 179.03 | kJ/mol | Joback Method |
| hf | -164.97 | kJ/mol | Joback Method |
| hfus | 21.69 | kJ/mol | Joback Method |
| hvap | 50.71 | kJ/mol | Joback Method |
| log10ws | -4.63 | | Crippen Method |
| logp | 4.581 | | Crippen Method |
| mcvol | 191.890 | ml/mol | McGowan Method |
| pc | 1921.98 | kPa | Joback Method |
| ripol | 1705.00 | | NIST Webbook |
| tb | 576.33 | K | Joback Method |
| tc | 791.72 | K | Joback Method |
| tf | 287.93 | K | Joback Method |
| vc | 0.723 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 503.29 | J/molxK | 576.33 | Joback Method |
| cpg | 526.08 | J/molxK | 612.23 | Joback Method |
| cpg | 547.54 | J/molxK | 648.13 | Joback Method |
| cpg | 567.74 | J/molxK | 684.03 | Joback Method |
| cpg | 586.71 | J/molxK | 719.93 | Joback Method |
| cpg | 604.51 | J/molxK | 755.83 | Joback Method |
| cpg | 621.19 | J/molxK | 791.72 | Joback Method |
| dvisc | 0.0020754 | Paxs | 287.93 | Joback Method |
| dvisc | 0.0012375 | Paxs | 336.00 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0008398 | Paxs | 384.06 | Joback Method |
| dvisc | 0.0006213 | Paxs | 432.13 | Joback Method |
| dvisc | 0.0004882 | Paxs | 480.20 | Joback Method |
| dvisc | 0.0004008 | Paxs | 528.26 | Joback Method |
| dvisc | 0.0003401 | Paxs | 576.33 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R438565&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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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

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