

Pentadecane, 7-ethyl-6-pentyl

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|-----------------------------|---|
| Inchi: | InChI=1S/C22H46/c1-5-9-12-13-14-17-18-21(8-4)22(19-15-10-6-2)20-16-11-7-3/h21-22H |
| InchiKey: | JPBRUFIBHQUGC-UHFFFAOYSA-N |
| Formula: | C22H46 |
| SMILES: | CCCCCCCC(CC)C(CCCCC)CCCC |
| Mol. weight [g/mol]: | 310.60 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 129.48 | kJ/mol | Joback Method |
| hf | -507.97 | kJ/mol | Joback Method |
| hfus | 45.69 | kJ/mol | Joback Method |
| hvap | 63.79 | kJ/mol | Joback Method |
| log10ws | -8.55 | | Crippen Method |
| logp | 8.540 | | Crippen Method |
| mvol | 320.840 | ml/mol | McGowan Method |
| pc | 910.53 | kPa | Joback Method |
| rinpol | 1946.00 | | NIST Webbook |
| tb | 701.88 | K | Joback Method |
| tc | 868.08 | K | Joback Method |
| tf | 307.70 | K | Joback Method |
| vc | 1.256 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 962.75 | J/molxK | 701.88 | Joback Method |
| cpg | 984.94 | J/molxK | 729.58 | Joback Method |
| cpg | 1006.16 | J/molxK | 757.28 | Joback Method |
| cpg | 1026.44 | J/molxK | 784.98 | Joback Method |
| cpg | 1045.81 | J/molxK | 812.68 | Joback Method |
| cpg | 1064.30 | J/molxK | 840.38 | Joback Method |
| cpg | 1081.95 | J/molxK | 868.08 | Joback Method |
| dvisc | 0.0057276 | Paxs | 307.70 | Joback Method |
| dvisc | 0.0014050 | Paxs | 373.40 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0005248 | Paxs | 439.09 | Joback Method |
| dvisc | 0.0002533 | Paxs | 504.79 | Joback Method |
| dvisc | 0.0001446 | Paxs | 570.49 | Joback Method |
| dvisc | 0.0000927 | Paxs | 636.18 | Joback Method |
| dvisc | 0.0000646 | Paxs | 701.88 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R9615&Units=SI |

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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<https://www.chemeo.com/cid/72-418-8/Pentadecane-7-ethyl-6-pentyl.pdf>

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