

Hexadecane, 6-heptyl

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|-----------------------------|---|
| Inchi: | InChI=1S/C23H48/c1-4-7-10-12-13-14-16-19-22-23(20-17-9-6-3)21-18-15-11-8-5-2/h23H |
| InchiKey: | KEKNVELWDFEQQX-UHFFFAOYSA-N |
| Formula: | C23H48 |
| SMILES: | CCCCCCCCCCC(CCCCC)CCCCCCC |
| Mol. weight [g/mol]: | 324.63 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 140.34 | kJ/mol | Joback Method |
| hf | -523.33 | kJ/mol | Joback Method |
| hfus | 51.80 | kJ/mol | Joback Method |
| hvap | 66.40 | kJ/mol | Joback Method |
| log10ws | -9.21 | | Crippen Method |
| logp | 9.074 | | Crippen Method |
| mvol | 334.930 | ml/mol | McGowan Method |
| pc | 855.96 | kPa | Joback Method |
| rinpol | 2166.00 | | NIST Webbook |
| rinpol | 2166.00 | | NIST Webbook |
| tb | 725.20 | K | Joback Method |
| tc | 892.42 | K | Joback Method |
| tf | 333.97 | K | Joback Method |
| vc | 1.317 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1024.67 | J/molxK | 725.20 | Joback Method |
| cpg | 1047.11 | J/molxK | 753.07 | Joback Method |
| cpg | 1068.56 | J/molxK | 780.94 | Joback Method |
| cpg | 1089.04 | J/molxK | 808.81 | Joback Method |
| cpg | 1108.60 | J/molxK | 836.68 | Joback Method |
| cpg | 1127.28 | J/molxK | 864.55 | Joback Method |
| cpg | 1145.09 | J/molxK | 892.42 | Joback Method |
| dvisc | 0.0035428 | Paxs | 333.97 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0010359 | Paxs | 399.17 | Joback Method |
| dvisc | 0.0004278 | Paxs | 464.38 | Joback Method |
| dvisc | 0.0002197 | Paxs | 529.59 | Joback Method |
| dvisc | 0.0001306 | Paxs | 594.79 | Joback Method |
| dvisc | 0.0000860 | Paxs | 659.99 | Joback Method |
| dvisc | 0.0000611 | Paxs | 725.20 | 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=R47885&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| 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/73-667-1/Hexadecane-6-heptyl.pdf>

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