

Octadecane, 5-methyl-

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|-----------------------------|---|
| Other names: | 5-methyloctadecane |
| Inchi: | InChI=1S/C19H40/c1-4-6-8-9-10-11-12-13-14-15-16-18-19(3)17-7-5-2/h19H,4-18H2,1-3H |
| InchiKey: | FRVYSTFGTANOHG-UHFFFAOYSA-N |
| Formula: | C19H40 |
| SMILES: | CCCCCCCCCCCCCCC(C)CCCC |
| Mol. weight [g/mol]: | 268.52 |
| CAS: | 25117-35-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| gf | 106.66 | kJ/mol | Joback Method |
| hf | -440.77 | kJ/mol | Joback Method |
| hfus | 41.44 | kJ/mol | Joback Method |
| hvap | 57.50 | kJ/mol | Joback Method |
| log10ws | -7.53 | | Crippen Method |
| logp | 7.514 | | Crippen Method |
| mcvol | 278.570 | ml/mol | McGowan Method |
| pc | 1086.35 | kPa | Joback Method |
| rinpol | 1853.00 | | NIST Webbook |
| rinpol | 1854.00 | | NIST Webbook |
| rinpol | 1853.00 | | NIST Webbook |
| rinpol | 1853.60 | | NIST Webbook |
| tb | 633.68 | K | Joback Method |
| tc | 794.96 | K | Joback Method |
| tf | 260.00 ± 3.00 | K | NIST Webbook |
| vc | 1.093 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 781.70 | J/mol×K | 633.68 | Joback Method |
| cpg | 802.48 | J/mol×K | 660.56 | Joback Method |
| cpg | 822.41 | J/mol×K | 687.44 | Joback Method |
| cpg | 841.51 | J/mol×K | 714.32 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 859.82 | J/mol×K | 741.20 | Joback Method |
| cpg | 877.35 | J/mol×K | 768.08 | Joback Method |
| cpg | 894.13 | J/mol×K | 794.96 | Joback Method |
| dvisc | 0.0057089 | Paxs | 288.89 | Joback Method |
| dvisc | 0.0016729 | Paxs | 346.36 | Joback Method |
| dvisc | 0.0006952 | Paxs | 403.82 | Joback Method |
| dvisc | 0.0003595 | Paxs | 461.29 | Joback Method |
| dvisc | 0.0002152 | Paxs | 518.75 | Joback Method |
| dvisc | 0.0001427 | Paxs | 576.22 | Joback Method |
| dvisc | 0.0001019 | Paxs | 633.68 | Joback Method |
| hvapt | 63.80 | kJ/mol | 520.00 | NIST Webbook |

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=C25117355&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 |
| hvapt: | Enthalpy of vaporization at a given temperature |
| 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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