

Hexadecane, 8,9-diethyl

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|----------------------|---|
| Inchi: | InChI=1S/C20H42/c1-5-9-11-13-15-17-19(7-3)20(8-4)18-16-14-12-10-6-2/h19-20H,5-18H |
| InchiKey: | BTGJAUOCHPVGFE-UHFFFAOYSA-N |
| Formula: | C20H42 |
| SMILES: | CCCCCCCC(CC)C(CC)CCCCCCC |
| Mol. weight [g/mol]: | 282.55 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 112.64 | kJ/mol | Joback Method |
| hf | -466.69 | kJ/mol | Joback Method |
| hfus | 40.51 | kJ/mol | Joback Method |
| hvap | 59.34 | kJ/mol | Joback Method |
| log10ws | -7.71 | | Crippen Method |
| logp | 7.760 | | Crippen Method |
| mcvol | 292.660 | ml/mol | McGowan Method |
| pc | 1025.97 | kPa | Joback Method |
| rinsol | 1811.00 | | NIST Webbook |
| tb | 656.12 | K | Joback Method |
| tc | 819.90 | K | Joback Method |
| tf | 285.16 | K | Joback Method |
| vc | 1.143 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 841.15 | J/molxK | 656.12 | Joback Method |
| cpg | 862.59 | J/molxK | 683.42 | Joback Method |
| cpg | 883.13 | J/molxK | 710.71 | Joback Method |
| cpg | 902.79 | J/molxK | 738.01 | Joback Method |
| cpg | 921.59 | J/molxK | 765.31 | Joback Method |
| cpg | 939.58 | J/molxK | 792.60 | Joback Method |
| cpg | 956.77 | J/molxK | 819.90 | Joback Method |
| dvisc | 0.0075349 | Paxs | 285.16 | Joback Method |
| dvisc | 0.0018250 | Paxs | 346.99 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0006788 | Paxs | 408.81 | Joback Method |
| dvisc | 0.0003274 | Paxs | 470.64 | Joback Method |
| dvisc | 0.0001870 | Paxs | 532.47 | Joback Method |
| dvisc | 0.0001200 | Paxs | 594.29 | Joback Method |
| dvisc | 0.0000838 | Paxs | 656.12 | 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=R9275&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/12-542-6/Hexadecane-8-9-diethyl.pdf>

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