

Dodecane, 5-butyl-6-ethyl

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|-----------------------------|---|
| Inchi: | InChI=1S/C18H38/c1-5-9-12-13-16-17(8-4)18(14-10-6-2)15-11-7-3/h17-18H,5-16H2,1-4H |
| InchiKey: | JXACHSBKZJSUFZ-UHFFFAOYSA-N |
| Formula: | C18H38 |
| SMILES: | CCCCCCC(CC)C(CCCC)CCCC |
| Mol. weight [g/mol]: | 254.49 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 95.80 | kJ/mol | Joback Method |
| hf | -425.41 | kJ/mol | Joback Method |
| hfus | 35.33 | kJ/mol | Joback Method |
| hvap | 54.89 | kJ/mol | Joback Method |
| log10ws | -6.87 | | Crippen Method |
| logp | 6.980 | | Crippen Method |
| mcvol | 264.480 | ml/mol | McGowan Method |
| pc | 1164.84 | kPa | Joback Method |
| rinsol | 1582.00 | | NIST Webbook |
| tb | 610.36 | K | Joback Method |
| tc | 773.50 | K | Joback Method |
| tf | 262.62 | K | Joback Method |
| vc | 1.032 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 724.07 | J/molxK | 610.36 | Joback Method |
| cpg | 819.32 | J/molxK | 746.31 | Joback Method |
| cpg | 801.88 | J/molxK | 719.12 | Joback Method |
| cpg | 783.65 | J/molxK | 691.93 | Joback Method |
| cpg | 764.63 | J/molxK | 664.74 | Joback Method |
| cpg | 744.77 | J/molxK | 637.55 | Joback Method |
| cpg | 836.01 | J/molxK | 773.50 | Joback Method |
| dvisc | 0.0001069 | Paxs | 610.36 | Joback Method |
| dvisc | 0.0001529 | Paxs | 552.40 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002378 | Paxs | 494.45 | Joback Method |
| dvisc | 0.0004158 | Paxs | 436.49 | Joback Method |
| dvisc | 0.0008629 | Paxs | 378.53 | Joback Method |
| dvisc | 0.0023312 | Paxs | 320.58 | Joback Method |
| dvisc | 0.0097660 | Paxs | 262.62 | 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=R8978&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/54-362-0/Dodecane-5-butyl-6-ethyl.pdf>

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