

Nonanoic acid, tridecyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C22H44O2/c1-3-5-7-9-11-12-13-14-15-17-19-21-24-22(23)20-18-16-10-8-6-4-2 |
| InchiKey: | VJWYCPPQGHETCD-UHFFFAOYSA-N |
| Formula: | C22H44O2 |
| SMILES: | CCCCCCCCCCCCOC(=O)CCCCCCCC |
| Mol. weight [g/mol]: | 340.58 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -99.56 | kJ/mol | Joback Method |
| hf | -742.21 | kJ/mol | Joback Method |
| hfus | 55.52 | kJ/mol | Joback Method |
| hvap | 73.72 | kJ/mol | Joback Method |
| log10ws | -7.89 | | Crippen Method |
| logp | 7.591 | | Crippen Method |
| mcvol | 328.280 | ml/mol | McGowan Method |
| pc | 927.24 | kPa | Joback Method |
| rinpola | 2372.00 | | NIST Webbook |
| tb | 779.05 | K | Joback Method |
| tc | 955.69 | K | Joback Method |
| tf | 409.86 | K | Joback Method |
| vc | 1.292 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1031.01 | J/molxK | 779.05 | Joback Method |
| cpg | 1124.02 | J/molxK | 926.25 | Joback Method |
| cpg | 1107.35 | J/molxK | 896.81 | Joback Method |
| cpg | 1089.74 | J/molxK | 867.37 | Joback Method |
| cpg | 1071.17 | J/molxK | 837.93 | Joback Method |
| cpg | 1051.60 | J/molxK | 808.49 | Joback Method |
| cpg | 1139.78 | J/molxK | 955.69 | Joback Method |
| dvisc | 0.0000557 | Paxs | 779.05 | Joback Method |
| dvisc | 0.0000754 | Paxs | 717.52 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0001080 | Paxs | 655.99 | Joback Method |
| dvisc | 0.0001666 | Paxs | 594.45 | Joback Method |
| dvisc | 0.0002843 | Paxs | 532.92 | Joback Method |
| dvisc | 0.0005575 | Paxs | 471.39 | Joback Method |
| dvisc | 0.0013386 | Paxs | 409.86 | 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=U340280&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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/86-930-4/Nonanoic-acid-tridecyl-ester.pdf>

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