

Pelargonic acid, nonyl ester

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|-----------------------------|---|
| Other names: | nonyl nonan-1-oate |
| Inchi: | InChI=1S/C18H36O2/c1-3-5-7-9-11-13-15-17-20-18(19)16-14-12-10-8-6-4-2/h3-17H2,1-2 |
| InchiKey: | WWDHABCVIVMHKP-UHFFFAOYSA-N |
| Formula: | C18H36O2 |
| SMILES: | CCCCCCCCCOC(=O)CCCCCCCC |
| Mol. weight [g/mol]: | 284.48 |
| CAS: | 87310-12-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -133.24 | kJ/mol | Joback Method |
| hf | -659.65 | kJ/mol | Joback Method |
| hfus | 45.16 | kJ/mol | Joback Method |
| hvap | 64.82 | kJ/mol | Joback Method |
| log10ws | -6.22 | | Crippen Method |
| logp | 6.031 | | Crippen Method |
| mcvol | 271.920 | ml/mol | McGowan Method |
| pc | 1189.06 | kPa | Joback Method |
| tb | 687.53 | K | Joback Method |
| tc | 855.83 | K | Joback Method |
| tf | 364.78 | K | Joback Method |
| vc | 1.067 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 789.92 | J/molxK | 687.53 | Joback Method |
| cpg | 875.72 | J/molxK | 827.78 | Joback Method |
| cpg | 860.14 | J/molxK | 799.73 | Joback Method |
| cpg | 843.80 | J/molxK | 771.68 | Joback Method |
| cpg | 826.65 | J/molxK | 743.63 | Joback Method |
| cpg | 808.70 | J/molxK | 715.58 | Joback Method |
| cpg | 890.54 | J/molxK | 855.83 | Joback Method |
| dvisc | 0.0000953 | Paxs | 687.53 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001278 | Paxs | 633.74 | Joback Method |
| dvisc | 0.0001809 | Paxs | 579.95 | Joback Method |
| dvisc | 0.0002749 | Paxs | 526.15 | Joback Method |
| dvisc | 0.0004595 | Paxs | 472.36 | Joback Method |
| dvisc | 0.0008765 | Paxs | 418.57 | Joback Method |
| dvisc | 0.0020226 | Paxs | 364.78 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C87310121&Units=SI |
| 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 |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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