

# Nonanoic acid, 2,3-dimethylphenyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C17H26O2/c1-4-5-6-7-8-9-13-17(18)19-16-12-10-11-14(2)15(16)3/h10-12H,4-9 |
| <b>InchiKey:</b>            | QCWAARQRPVKNFR-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C17H26O2  |
| <b>SMILES:</b>              | CCCCCCCCC(=O)Oc1cccc(C)c1C  |
| <b>Mol. weight [g/mol]:</b> | 262.39  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -48.51  | kJ/mol               | Joback Method  |
| hf            | -425.42 | kJ/mol               | Joback Method  |
| hfus          | 35.84   | kJ/mol               | Joback Method  |
| hvap          | 66.19   | kJ/mol               | Joback Method  |
| log10ws       | -5.67   |                      | Crippen Method |
| logp          | 4.959   |                      | Crippen Method |
| mcvol         | 234.070 | ml/mol               | McGowan Method |
| pc            | 1596.17 | kPa                  | Joback Method  |
| rinpola       | 2013.00 |                      | NIST Webbook   |
| tb            | 701.29  | K                    | Joback Method  |
| tc            | 896.38  | K                    | Joback Method  |
| tf            | 404.97  | K                    | Joback Method  |
| vc            | 0.903   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 654.31    | J/molxK | 701.29          | Joback Method |
| cpg           | 671.53    | J/molxK | 733.80          | Joback Method |
| cpg           | 687.82    | J/molxK | 766.32          | Joback Method |
| cpg           | 703.19    | J/molxK | 798.83          | Joback Method |
| cpg           | 717.67    | J/molxK | 831.35          | Joback Method |
| cpg           | 731.28    | J/molxK | 863.86          | Joback Method |
| cpg           | 744.04    | J/molxK | 896.38          | Joback Method |
| dvisc         | 0.0010807 | Paxs    | 404.97          | Joback Method |
| dvisc         | 0.0005971 | Paxs    | 454.36          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003706 | Paxs | 503.74 | Joback Method |
| dvisc | 0.0002505 | Paxs | 553.13 | Joback Method |
| dvisc | 0.0001805 | Paxs | 602.52 | Joback Method |
| dvisc | 0.0001367 | Paxs | 651.90 | Joback Method |
| dvisc | 0.0001077 | Paxs | 701.29 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360671&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360671&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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