

# Adipic acid, 4-heptyl pentadecyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C28H54O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-20-25-31-27(29)23-18-19-24- |
| <b>InchiKey:</b>            | JKUWYSRMLWHQKJ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C28H54O4   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(CCC)CCC  |
| <b>Mol. weight [g/mol]:</b> | 454.73   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -285.40  | kJ/mol               | Joback Method  |
| hf            | -1116.13 | kJ/mol               | Joback Method  |
| hfus          | 70.33    | kJ/mol               | Joback Method  |
| hvap          | 95.85    | kJ/mol               | Joback Method  |
| log10ws       | -9.38    |                      | Crippen Method |
| logp          | 8.693    |                      | Crippen Method |
| mvol          | 420.260  | ml/mol               | McGowan Method |
| pc            | 690.34   | kPa                  | Joback Method  |
| rinpol        | 3000.00  |                      | NIST Webbook   |
| rinpol        | 3000.00  |                      | NIST Webbook   |
| tb            | 992.18   | K                    | Joback Method  |
| tc            | 1230.25  | K                    | Joback Method  |
| tf            | 534.64   | K                    | Joback Method  |
| vc            | 1.645    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1474.86   | J/molxK | 992.18          | Joback Method |
| cpg           | 1497.34   | J/molxK | 1031.86         | Joback Method |
| cpg           | 1517.80   | J/molxK | 1071.54         | Joback Method |
| cpg           | 1536.31   | J/molxK | 1111.22         | Joback Method |
| cpg           | 1552.94   | J/molxK | 1150.90         | Joback Method |
| cpg           | 1567.75   | J/molxK | 1190.58         | Joback Method |
| cpg           | 1580.84   | J/molxK | 1230.25         | Joback Method |
| dvisc         | 0.0003555 | Paxs    | 534.64          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001491 | Paxs | 610.90 | Joback Method |
| dvisc | 0.0000759 | Paxs | 687.15 | Joback Method |
| dvisc | 0.0000442 | Paxs | 763.41 | Joback Method |
| dvisc | 0.0000284 | Paxs | 839.67 | Joback Method |
| dvisc | 0.0000196 | Paxs | 915.92 | Joback Method |
| dvisc | 0.0000144 | Paxs | 992.18 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=U349749&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349749&amp;Units=SI</a> |
| <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>                                 |

## 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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