

# Succinic acid, 2-hexyl nonadecyl ester

Inchi:

InChI=1S/C29H56O4/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-26-32-28(30)

InchiKey:

RDSRIZZUWNEIDY-UHFFFAOYSA-N

Formula:

C29H56O4

SMILES:

CCCCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OC(C)CCCC

Mol. weight [g/mol]:

468.75

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -276.98  | kJ/mol  | Joback Method  |
| hf            | -1136.77 | kJ/mol  | Joback Method  |
| hfus          | 72.92    | kJ/mol  | Joback Method  |
| hvap          | 98.07    | kJ/mol  | Joback Method  |
| log10ws       | -9.80    |         | Crippen Method |
| logp          | 9.083    |         | Crippen Method |
| mcvol         | 434.350  | ml/mol  | McGowan Method |
| pc            | 656.79   | kPa     | Joback Method  |
| rinpol        | 3140.00  |         | NIST Webbook   |
| rinpol        | 3140.00  |         | NIST Webbook   |
| tb            | 1015.06  | K       | Joback Method  |
| tc            | 1265.21  | K       | Joback Method  |
| tf            | 545.91   | K       | Joback Method  |
| vc            | 1.702    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1539.99   | J/mol×K | 1015.06         | Joback Method |
| cpg           | 1563.19   | J/mol×K | 1056.75         | Joback Method |
| cpg           | 1584.14   | J/mol×K | 1098.44         | Joback Method |
| cpg           | 1602.93   | J/mol×K | 1140.13         | Joback Method |
| cpg           | 1619.67   | J/mol×K | 1181.83         | Joback Method |
| cpg           | 1634.42   | J/mol×K | 1223.52         | Joback Method |
| cpg           | 1647.29   | J/mol×K | 1265.21         | Joback Method |
| dvisc         | 0.0003091 | Pa×s    | 545.91          | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0001288 | Pa×s | 624.10  | Joback Method |
| dvisc | 0.0000652 | Pa×s | 702.29  | Joback Method |
| dvisc | 0.0000378 | Pa×s | 780.49  | Joback Method |
| dvisc | 0.0000242 | Pa×s | 858.68  | Joback Method |
| dvisc | 0.0000167 | Pa×s | 936.87  | Joback Method |
| dvisc | 0.0000122 | Pa×s | 1015.06 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U349567&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349567&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>                                     |

## 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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