

# Sebacic acid, heptyl hexyl ester

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C23H44O4/c1-3-5-7-13-17-21-27-23(25)19-15-12-10-9-11-14-18-22(24)26-20- |
| InchiKey:            | OTPXBFLOWKPACJ-UHFFFAOYSA-N                                                      |
| Formula:             | C23H44O4                                                                         |
| SMILES:              | CCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCC                                                |
| Mol. weight [g/mol]: | 384.59                                                                           |

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -325.06  | kJ/mol  | Joback Method  |
| hf            | -1007.65 | kJ/mol  | Joback Method  |
| hfus          | 60.90    | kJ/mol  | Joback Method  |
| hvap          | 85.10    | kJ/mol  | Joback Method  |
| log10ws       | -7.18    |         | Crippen Method |
| logp          | 6.744    |         | Crippen Method |
| mcvol         | 349.810  | ml/mol  | McGowan Method |
| pc            | 899.64   | kPa     | Joback Method  |
| rinpol        | 2723.00  |         | NIST Webbook   |
| tb            | 878.22   | K       | Joback Method  |
| tc            | 1075.46  | K       | Joback Method  |
| tf            | 493.29   | K       | Joback Method  |
| vc            | 1.371    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1154.52   | J/mol×K | 878.22          | Joback Method |
| cpg           | 1174.19   | J/mol×K | 911.09          | Joback Method |
| cpg           | 1192.56   | J/mol×K | 943.97          | Joback Method |
| cpg           | 1209.66   | J/mol×K | 976.84          | Joback Method |
| cpg           | 1225.52   | J/mol×K | 1009.71         | Joback Method |
| cpg           | 1240.17   | J/mol×K | 1042.59         | Joback Method |
| cpg           | 1253.64   | J/mol×K | 1075.46         | Joback Method |
| dvisc         | 0.0005944 | Pa×s    | 493.29          | Joback Method |
| dvisc         | 0.0002809 | Pa×s    | 557.44          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001550 | Pa×s | 621.60 | Joback Method |
| dvisc | 0.0000955 | Pa×s | 685.75 | Joback Method |
| dvisc | 0.0000640 | Pa×s | 749.91 | Joback Method |
| dvisc | 0.0000457 | Pa×s | 814.07 | Joback Method |
| dvisc | 0.0000342 | Pa×s | 878.22 | 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=U354250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354250&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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