

# Carbonic acid, di(decyl) ester

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | di-n-decyl carbonate<br>dicapryl carbonate<br>didecyl carbonate                   |
| Inchi:               | InChI=1S/C21H42O3/c1-3-5-7-9-11-13-15-17-19-23-21(22)24-20-18-16-14-12-10-8-6-4-2 |
| InchiKey:            | ZEBJPYUECLCDRQ-UHFFFAOYSA-N                                                       |
| Formula:             | C21H42O3                                                                          |
| SMILES:              | CCCCCCCCCCCCOC(=O)CCCCCCCCCCCC                                                    |
| Mol. weight [g/mol]: | 342.56                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source                                                                                                 |
|---------------|---------|---------|--------------------------------------------------------------------------------------------------------|
| gf            | -212.98 | kJ/mol  | Joback Method                                                                                          |
| hf            | -853.79 | kJ/mol  | Joback Method                                                                                          |
| hfus          | 54.12   | kJ/mol  | Joback Method                                                                                          |
| hvap          | 73.91   | kJ/mol  | Joback Method                                                                                          |
| log10ws       | -7.54   |         | Crippen Method                                                                                         |
| logp          | 7.421   |         | Crippen Method                                                                                         |
| mcvol         | 320.060 | ml/mol  | McGowan Method                                                                                         |
| pc            | 973.52  | kPa     | Joback Method                                                                                          |
| rinpol        | 2328.00 |         | NIST Webbook                                                                                           |
| tb            | 778.59  | K       | Joback Method                                                                                          |
| tc            | 955.33  | K       | Joback Method                                                                                          |
| tf            | 272.15  | K       | The manufacture of organic carbonate-poly(methyl ethylacrylate) nanowebs with thermal buffering effect |
| vc            | 1.254   | m3/kmol | Joback Method                                                                                          |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1002.70 | J/mol×K | 778.59          | Joback Method |
| cpg           | 1022.68 | J/mol×K | 808.05          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 1041.64   | J/mol×K | 837.50 | Joback Method |
| cpg   | 1059.60   | J/mol×K | 866.96 | Joback Method |
| cpg   | 1076.58   | J/mol×K | 896.41 | Joback Method |
| cpg   | 1092.59   | J/mol×K | 925.87 | Joback Method |
| cpg   | 1107.66   | J/mol×K | 955.33 | Joback Method |
| dvisc | 0.0010020 | Pa×s    | 420.82 | Joback Method |
| dvisc | 0.0004416 | Pa×s    | 480.45 | Joback Method |
| dvisc | 0.0002332 | Pa×s    | 540.08 | Joback Method |
| dvisc | 0.0001398 | Pa×s    | 599.70 | Joback Method |
| dvisc | 0.0000920 | Pa×s    | 659.33 | Joback Method |
| dvisc | 0.0000649 | Pa×s    | 718.96 | Joback Method |
| dvisc | 0.0000482 | Pa×s    | 778.59 | Joback Method |

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

The manufacture of organic carbonate-poly(methyl ethylacrylate) nanobubbles with thermal buffering effect:

<https://www.doi.org/10.1016/j.tca.2017.10.003>

McGowan Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U383159&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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                   |

**vc:** Critical Volume

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