

# Carbonic acid, (1R)-(-)-menthyl undecyl ester

Inchi:

lnchl=1S/C22H42O3/c1-5-6-7-8-9-10-11-12-13-16-24-22(23)25-21-17-20(18(2)3)15-14-1

InchiKey:

VCDCQWUJGITWQD-UHFFFAOYSA-N

Formula:

C22H42O3

SMILES:

CCCCCCCCCCCCOC(=O)OC1CC(C(C)C)CCC1C

Mol. weight [g/mol]:

354.57

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -197.97 | kJ/mol  | Joback Method  |
| hf            | -866.07 | kJ/mol  | Joback Method  |
| hfus          | 47.16   | kJ/mol  | Joback Method  |
| hvap          | 75.56   | kJ/mol  | Joback Method  |
| log10ws       | -7.24   |         | Crippen Method |
| logp          | 7.131   |         | Crippen Method |
| mcvol         | 323.290 | ml/mol  | McGowan Method |
| pc            | 1005.26 | kPa     | Joback Method  |
| rinpol        | 2390.00 |         | NIST Webbook   |
| rinpol        | 2390.00 |         | NIST Webbook   |
| tb            | 811.24  | K       | Joback Method  |
| tc            | 1001.53 | K       | Joback Method  |
| tf            | 415.99  | K       | Joback Method  |
| vc            | 1.234   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1069.21   | J/mol×K | 811.24          | Joback Method |
| cpg           | 1091.10   | J/mol×K | 842.96          | Joback Method |
| cpg           | 1111.59   | J/mol×K | 874.67          | Joback Method |
| cpg           | 1130.71   | J/mol×K | 906.39          | Joback Method |
| cpg           | 1148.47   | J/mol×K | 938.10          | Joback Method |
| cpg           | 1164.89   | J/mol×K | 969.82          | Joback Method |
| cpg           | 1179.98   | J/mol×K | 1001.53         | Joback Method |
| dvisc         | 0.0012691 | Pa×s    | 415.99          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0005509 | Pa×s | 481.87 | Joback Method |
| dvisc | 0.0002923 | Pa×s | 547.74 | Joback Method |
| dvisc | 0.0001777 | Pa×s | 613.62 | Joback Method |
| dvisc | 0.0001190 | Pa×s | 679.49 | Joback Method |
| dvisc | 0.0000855 | Pa×s | 745.37 | Joback Method |
| dvisc | 0.0000649 | Pa×s | 811.24 | 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=U392440&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392440&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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