

# Allyl tricosanoate

Inchi:

InChI=1S/C26H50O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26

InchiKey:

CLRFJBXIZDMMBQ-UHFFFAOYSA-N

Formula:

C26H50O2

SMILES:

C=CCOC(=O)CCCCCCCCCCCCCCCCCCCCC

Mol. weight [g/mol]:

394.67

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 21.96   | kJ/mol  | Joback Method  |
| hf            | -699.34 | kJ/mol  | Joback Method  |
| hfus          | 64.60   | kJ/mol  | Joback Method  |
| hvap          | 81.96   | kJ/mol  | Joback Method  |
| log10ws       | -9.42   |         | Crippen Method |
| logp          | 8.928   |         | Crippen Method |
| mcvol         | 380.340 | ml/mol  | McGowan Method |
| pc            | 760.58  | kPa     | Joback Method  |
| rinpol        | 2744.00 |         | NIST Webbook   |
| tb            | 867.25  | K       | Joback Method  |
| tc            | 1062.66 | K       | Joback Method  |
| tf            | 453.18  | K       | Joback Method  |
| vc            | 1.496   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1256.75   | J/mol×K | 867.25          | Joback Method |
| cpg           | 1279.01   | J/mol×K | 899.82          | Joback Method |
| cpg           | 1300.00   | J/mol×K | 932.39          | Joback Method |
| cpg           | 1319.76   | J/mol×K | 964.96          | Joback Method |
| cpg           | 1338.34   | J/mol×K | 997.53          | Joback Method |
| cpg           | 1355.79   | J/mol×K | 1030.10         | Joback Method |
| cpg           | 1372.17   | J/mol×K | 1062.66         | Joback Method |
| dvisc         | 0.0008402 | Pa×s    | 453.18          | Joback Method |
| dvisc         | 0.0003441 | Pa×s    | 522.19          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001735 | Pa×s | 591.20 | Joback Method |
| dvisc | 0.0001010 | Pa×s | 660.22 | Joback Method |
| dvisc | 0.0000651 | Pa×s | 729.23 | Joback Method |
| dvisc | 0.0000453 | Pa×s | 798.24 | Joback Method |
| dvisc | 0.0000334 | Pa×s | 867.25 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                     |
| <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=R541176&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R541176&amp;Units=SI</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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