

# Docosyl, isovalerate

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C27H54O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-29 |
| <b>InchiKey:</b>            | OFRPMAQLXIEORX-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C27H54O2   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCCCCCCOC(=O)CC(C)C  |
| <b>Mol. weight [g/mol]:</b> | 410.72   |
| <b>CAS:</b>                 | 202659-53-8  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -59.90  | kJ/mol  | Joback Method  |
| hf            | -850.69 | kJ/mol  | Joback Method  |
| hfus          | 64.95   | kJ/mol  | Joback Method  |
| hvap          | 84.46   | kJ/mol  | Joback Method  |
| log10ws       | -9.75   |         | Crippen Method |
| logp          | 9.398   |         | Crippen Method |
| mcvol         | 398.730 | ml/mol  | McGowan Method |
| pc            | 708.84  | kPa     | Joback Method  |
| rinpol        | 2841.40 |         | NIST Webbook   |
| rinpol        | 2841.40 |         | NIST Webbook   |
| tb            | 893.01  | K       | Joback Method  |
| tc            | 1096.23 | K       | Joback Method  |
| tf            | 451.21  | K       | Joback Method  |
| vc            | 1.565   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1350.92 | J/molxK | 893.01          | Joback Method |
| cpg           | 1454.55 | J/molxK | 1062.36         | Joback Method |
| cpg           | 1436.51 | J/molxK | 1028.49         | Joback Method |
| cpg           | 1417.19 | J/molxK | 994.62          | Joback Method |
| cpg           | 1396.52 | J/molxK | 960.75          | Joback Method |
| cpg           | 1374.45 | J/molxK | 926.88          | Joback Method |
| cpg           | 1471.36 | J/molxK | 1096.23         | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000245 | Paxs | 893.01 | Joback Method |
| dvisc | 0.0000339 | Paxs | 819.38 | Joback Method |
| dvisc | 0.0000503 | Paxs | 745.74 | Joback Method |
| dvisc | 0.0000811 | Paxs | 672.11 | Joback Method |
| dvisc | 0.0001473 | Paxs | 598.48 | Joback Method |
| dvisc | 0.0003163 | Paxs | 524.84 | Joback Method |
| dvisc | 0.0008713 | Paxs | 451.21 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C202659538&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C202659538&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>                               |

## 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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