

# Diamyl succinate

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | dipentyl succinate<br>dipentyl butanedioate                                   |
| <b>Inchi:</b>               | InChI=1S/C14H26O4/c1-3-5-7-11-17-13(15)9-10-14(16)18-12-8-6-4-2/h3-12H2,1-2H3 |
| <b>InchiKey:</b>            | JYCRKSLWSLBYLT-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C14H26O4  |
| <b>SMILES:</b>              | CCCCCOC(=O)CCC(=O)OCCCCC  |
| <b>Mol. weight [g/mol]:</b> | 258.35  |
| <b>CAS:</b>                 | 645-69-2  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -400.84 | kJ/mol  | Joback Method  |
| hf            | -821.89 | kJ/mol  | Joback Method  |
| hfus          | 37.59   | kJ/mol  | Joback Method  |
| hvap          | 65.07   | kJ/mol  | Joback Method  |
| log10ws       | -3.41   |         | Crippen Method |
| logp          | 3.233   |         | Crippen Method |
| mcvol         | 223.000 | ml/mol  | McGowan Method |
| pc            | 1639.10 | kPa     | Joback Method  |
| rinpol        | 1740.00 |         | NIST Webbook   |
| rinpol        | 1718.00 |         | NIST Webbook   |
| tb            | 672.30  | K       | Joback Method  |
| tc            | 848.26  | K       | Joback Method  |
| tf            | 391.86  | K       | Joback Method  |
| vc            | 0.868   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 622.19 | J/molxK | 672.30          | Joback Method |
| cpg           | 637.83 | J/molxK | 701.63          | Joback Method |
| cpg           | 652.75 | J/molxK | 730.95          | Joback Method |
| cpg           | 666.95 | J/molxK | 760.28          | Joback Method |
| cpg           | 680.44 | J/molxK | 789.61          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 693.22    | J/mol×K | 818.93 | Joback Method |
| cpg   | 705.29    | J/mol×K | 848.26 | Joback Method |
| dvisc | 0.0014859 | Paxs    | 391.86 | Joback Method |
| dvisc | 0.0007810 | Paxs    | 438.60 | Joback Method |
| dvisc | 0.0004646 | Paxs    | 485.34 | Joback Method |
| dvisc | 0.0003028 | Paxs    | 532.08 | Joback Method |
| dvisc | 0.0002115 | Paxs    | 578.82 | Joback Method |
| dvisc | 0.0001558 | Paxs    | 625.56 | Joback Method |
| dvisc | 0.0001198 | Paxs    | 672.30 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C645692&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C645692&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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