

# 2-pentacosene (E)

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C25H50/c1-3-5-7-9-11-13-15-17-19-21-23-25-24-22-20-18-16-14-12-10-8-6-4-2 |
| InchiKey:            | FBNVWVWQGXXNHZAR-HWKANZROSA-N  |
| Formula:             | C25H50   |
| SMILES:              | CC=CCCCCCCCCCCCCCCCCCCCCCC   |
| Mol. weight [g/mol]: | 350.66   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 239.84  | kJ/mol               | Joback Method  |
| hf            | -442.11 | kJ/mol               | Joback Method  |
| hfus          | 60.71   | kJ/mol               | Joback Method  |
| hvap          | 71.20   | kJ/mol               | Joback Method  |
| log10ws       | -10.14  |                      | Crippen Method |
| logp          | 9.775   |                      | Crippen Method |
| mcvol         | 358.810 | ml/mol               | McGowan Method |
| pc            | 786.39  | kPa                  | Joback Method  |
| rinpol        | 2506.00 |                      | NIST Webbook   |
| tb            | 775.56  | K                    | Joback Method  |
| tc            | 950.67  | K                    | Joback Method  |
| tf            | 366.43  | K                    | Joback Method  |
| vc            | 1.415   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1127.97   | J/molxK | 775.56          | Joback Method |
| cpg           | 1231.81   | J/molxK | 921.48          | Joback Method |
| cpg           | 1212.94   | J/molxK | 892.30          | Joback Method |
| cpg           | 1193.17   | J/molxK | 863.11          | Joback Method |
| cpg           | 1172.45   | J/molxK | 833.93          | Joback Method |
| cpg           | 1150.73   | J/molxK | 804.74          | Joback Method |
| cpg           | 1249.84   | J/molxK | 950.67          | Joback Method |
| dvisc         | 0.0000437 | Paxs    | 775.56          | Joback Method |
| dvisc         | 0.0000607 | Paxs    | 707.37          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000904 | Paxs | 639.18 | Joback Method |
| dvisc | 0.0001480 | Paxs | 570.99 | Joback Method |
| dvisc | 0.0002771 | Paxs | 502.81 | Joback Method |
| dvisc | 0.0006316 | Paxs | 434.62 | Joback Method |
| dvisc | 0.0019564 | Paxs | 366.43 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R205875&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R205875&amp;Units=SI</a> |
| <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>                     |

## 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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