

# Heneicosane, 11-phenyl-

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Other names:         | Benzene, (1-decylundecyl)-<br>11-Phenylheneicosane                                |
| Inchi:               | InChI=1S/C27H48/c1-3-5-7-9-11-13-15-18-22-26(27-24-20-17-21-25-27)23-19-16-14-12- |
| InchiKey:            | NDSAOEARRHEOPX-UHFFFAOYSA-N                                                       |
| Formula:             | C27H48                                                                            |
| SMILES:              | CCCCCCCCCCCC(CCCCCCCCCC)c1ccccc1                                                  |
| Mol. weight [g/mol]: | 372.67                                                                            |
| CAS:                 | 6703-80-6                                                                         |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 286.43        | kJ/mol  | Joback Method  |
| hf            | -369.36       | kJ/mol  | Joback Method  |
| hfus          | 56.20         | kJ/mol  | Joback Method  |
| hvap          | 77.58         | kJ/mol  | Joback Method  |
| log10ws       | -10.19        |         | Crippen Method |
| logp          | 9.832         |         | Crippen Method |
| mcvol         | 367.530       | ml/mol  | McGowan Method |
| pc            | 830.02        | kPa     | Joback Method  |
| tb            | 843.40        | K       | Joback Method  |
| tc            | 1034.84       | K       | Joback Method  |
| tf            | 293.95 ± 0.40 | K       | NIST Webbook   |
| tf            | 293.95 ± 0.50 | K       | NIST Webbook   |
| tt            | 266.90 ± 0.20 | K       | NIST Webbook   |
| vc            | 1.433         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1295.88 | J/mol×K | 1002.93         | Joback Method |
| cpg           | 1312.63 | J/mol×K | 1034.84         | Joback Method |
| cpg           | 1196.45 | J/mol×K | 843.40          | Joback Method |
| cpg           | 1218.65 | J/mol×K | 875.31          | Joback Method |
| cpg           | 1239.63 | J/mol×K | 907.21          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 1259.45   | J/mol×K | 939.12 | Joback Method |
| cpg   | 1278.18   | J/mol×K | 971.02 | Joback Method |
| dvisc | 0.0000355 | Pa×s    | 843.40 | Joback Method |
| dvisc | 0.0000493 | Pa×s    | 770.41 | Joback Method |
| dvisc | 0.0015021 | Pa×s    | 405.47 | Joback Method |
| dvisc | 0.0005000 | Pa×s    | 478.46 | Joback Method |
| dvisc | 0.0002227 | Pa×s    | 551.45 | Joback Method |
| dvisc | 0.0001198 | Pa×s    | 624.43 | Joback Method |
| dvisc | 0.0000734 | Pa×s    | 697.42 | Joback Method |
| hfust | 64.77     | kJ/mol  | 294.30 | NIST Webbook  |
| hvapt | 93.50     | kJ/mol  | 510.00 | NIST Webbook  |

## 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=C6703806&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6703806&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>hfust:</b>   | Enthalpy of fusion at a given temperature       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>tt:</b>      | Triple Point Temperature                        |

**vc:** Critical Volume

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