

# Benzene, (1-pentyloctyl)-

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | Tridecane, 6-phenyl-                                                               |
| Inchi:               | InChI=1S/C19H32/c1-3-5-7-8-11-15-18(14-10-6-4-2)19-16-12-9-13-17-19/h9,12-13,16-18 |
| InchiKey:            | OTSYFFDVDLHIKX-UHFFFAOYSA-N                                                        |
| Formula:             | C19H32                                                                             |
| SMILES:              | CCCCCCCC(CCCCC)c1ccccc1                                                            |
| Mol. weight [g/mol]: | 260.46                                                                             |
| CAS:                 | 4534-49-0                                                                          |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 219.07  | kJ/mol  | Joback Method  |
| hf            | -204.24 | kJ/mol  | Joback Method  |
| hfus          | 35.48   | kJ/mol  | Joback Method  |
| hvap          | 59.78   | kJ/mol  | Joback Method  |
| log10ws       | -6.84   |         | Crippen Method |
| logp          | 6.711   |         | Crippen Method |
| mcvol         | 254.810 | ml/mol  | McGowan Method |
| pc            | 1368.70 | kPa     | Joback Method  |
| rinpol        | 308.50  |         | NIST Webbook   |
| rinpol        | 1814.00 |         | NIST Webbook   |
| rinpol        | 1819.00 |         | NIST Webbook   |
| rinpol        | 1813.00 |         | NIST Webbook   |
| rinpol        | 1814.00 |         | NIST Webbook   |
| ripol         | 2015.00 |         | NIST Webbook   |
| tb            | 660.36  | K       | Joback Method  |
| tc            | 847.35  | K       | Joback Method  |
| tf            | 315.31  | K       | Joback Method  |
| vc            | 0.986   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 710.04 | J/mol×K | 660.36          | Joback Method |
| cpg           | 730.40 | J/mol×K | 691.52          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 749.69    | J/mol×K | 722.69 | Joback Method |
| cpg   | 767.96    | J/mol×K | 753.85 | Joback Method |
| cpg   | 785.26    | J/mol×K | 785.02 | Joback Method |
| cpg   | 801.63    | J/mol×K | 816.18 | Joback Method |
| cpg   | 817.11    | J/mol×K | 847.35 | Joback Method |
| dvisc | 0.0037196 | Pa×s    | 315.31 | Joback Method |
| dvisc | 0.0012862 | Pa×s    | 372.82 | Joback Method |
| dvisc | 0.0005907 | Pa×s    | 430.33 | Joback Method |
| dvisc | 0.0003259 | Pa×s    | 487.84 | Joback Method |
| dvisc | 0.0002039 | Pa×s    | 545.34 | Joback Method |
| dvisc | 0.0001395 | Pa×s    | 602.85 | Joback Method |
| dvisc | 0.0001019 | Pa×s    | 660.36 | 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=C4534490&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4534490&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>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |

**vc:** Critical Volume

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