

# Benzene, (1-heptyloctyl)-

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | Pentadecane, 8-phenyl-<br>8-phenylpentadecane                                      |
| Inchi:               | InChI=1S/C21H36/c1-3-5-7-9-12-16-20(17-13-10-8-6-4-2)21-18-14-11-15-19-21/h11,14-1 |
| InchiKey:            | RECLSKJUKJFZCW-UHFFFAOYSA-N                                                        |
| Formula:             | C21H36                                                                             |
| SMILES:              | CCCCCCCC(CCCCCC)c1ccccc1                                                           |
| Mol. weight [g/mol]: | 288.51                                                                             |
| CAS:                 | 4534-60-5                                                                          |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 235.91  | kJ/mol  | Joback Method  |
| hf            | -245.52 | kJ/mol  | Joback Method  |
| hfus          | 40.66   | kJ/mol  | Joback Method  |
| hvap          | 64.23   | kJ/mol  | Joback Method  |
| log10ws       | -7.68   |         | Crippen Method |
| logp          | 7.491   |         | Crippen Method |
| mcvol         | 282.990 | ml/mol  | McGowan Method |
| pc            | 1193.17 | kPa     | Joback Method  |
| tb            | 706.12  | K       | Joback Method  |
| tc            | 890.97  | K       | Joback Method  |
| tf            | 337.85  | K       | Joback Method  |
| vc            | 1.097   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 826.04 | J/mol×K | 706.12          | Joback Method |
| cpg           | 846.80 | J/mol×K | 736.93          | Joback Method |
| cpg           | 866.48 | J/mol×K | 767.74          | Joback Method |
| cpg           | 885.12 | J/mol×K | 798.54          | Joback Method |
| cpg           | 902.78 | J/mol×K | 829.35          | Joback Method |
| cpg           | 919.49 | J/mol×K | 860.16          | Joback Method |
| cpg           | 935.30 | J/mol×K | 890.97          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0030527 | Pa×s | 337.85 | Joback Method |
| dvisc | 0.0010434 | Pa×s | 399.23 | Joback Method |
| dvisc | 0.0004748 | Pa×s | 460.61 | Joback Method |
| dvisc | 0.0002600 | Pa×s | 521.99 | Joback Method |
| dvisc | 0.0001616 | Pa×s | 583.36 | Joback Method |
| dvisc | 0.0001100 | Pa×s | 644.74 | Joback Method |
| dvisc | 0.0000800 | Pa×s | 706.12 | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                           |
| <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=C4534605&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4534605&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>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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