

# Benzene, (1,1-dimethyldecyl)-

|                      |                                                                                     |
|----------------------|-------------------------------------------------------------------------------------|
| Other names:         | Undecane, 2-methyl-2-phenyl-(1,1-Dimethyldecyl)benzene<br>2-Methyl-2-phenylundecane |
| Inchi:               | InChI=1S/C18H30/c1-4-5-6-7-8-9-13-16-18(2,3)17-14-11-10-12-15-17/h10-12,14-15H,4-9  |
| InchiKey:            | FZUMQFUHECRZDF-UHFFFAOYSA-N                                                         |
| Formula:             | C18H30                                                                              |
| SMILES:              | CCCCCCCCCCC(C)(C)c1ccccc1                                                           |
| Mol. weight [g/mol]: | 246.43                                                                              |
| CAS:                 | 27854-40-6                                                                          |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 215.93  | kJ/mol  | Joback Method  |
| hf            | -187.07 | kJ/mol  | Joback Method  |
| hfus          | 29.00   | kJ/mol  | Joback Method  |
| hvap          | 56.64   | kJ/mol  | Joback Method  |
| log10ws       | -6.13   |         | Crippen Method |
| logp          | 6.105   |         | Crippen Method |
| mcvol         | 240.720 | ml/mol  | McGowan Method |
| pc            | 1483.85 | kPa     | Joback Method  |
| tb            | 634.69  | K       | Joback Method  |
| tc            | 829.36  | K       | Joback Method  |
| tf            | 321.46  | K       | Joback Method  |
| vc            | 0.924   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 655.85 | J/mol×K | 634.69          | Joback Method |
| cpg           | 676.44 | J/mol×K | 667.13          | Joback Method |
| cpg           | 695.86 | J/mol×K | 699.58          | Joback Method |
| cpg           | 714.16 | J/mol×K | 732.02          | Joback Method |
| cpg           | 731.42 | J/mol×K | 764.47          | Joback Method |
| cpg           | 747.69 | J/mol×K | 796.91          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 763.03    | J/mol×K | 829.36 | Joback Method |
| dvisc | 0.0035370 | Pa×s    | 321.46 | Joback Method |
| dvisc | 0.0013135 | Pa×s    | 373.67 | Joback Method |
| dvisc | 0.0006218 | Pa×s    | 425.87 | Joback Method |
| dvisc | 0.0003466 | Pa×s    | 478.07 | Joback Method |
| dvisc | 0.0002168 | Pa×s    | 530.28 | Joback Method |
| dvisc | 0.0001475 | Pa×s    | 582.48 | Joback Method |
| dvisc | 0.0001069 | Pa×s    | 634.69 | 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=C27854406&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27854406&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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