

# «alpha»-Isobutyldecalin

|                      |                                                                              |
|----------------------|------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C14H26/c1-11(2)10-13-8-5-7-12-6-3-4-9-14(12)13/h11-14H,3-10H2,1-2H3 |
| InchiKey:            | UGISRBVUOVJMIH-UHFFFAOYSA-N                                                  |
| Formula:             | C14H26                                                                       |
| SMILES:              | CC(C)CC1CCCC2CCCCC21                                                         |
| Mol. weight [g/mol]: | 194.36                                                                       |
| CAS:                 | 92369-83-0                                                                   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 129.95  | kJ/mol  | Joback Method  |
| hf            | -236.95 | kJ/mol  | Joback Method  |
| hfus          | 17.43   | kJ/mol  | Joback Method  |
| hvap          | 46.58   | kJ/mol  | Joback Method  |
| log10ws       | -4.51   |         | Crippen Method |
| logp          | 4.639   |         | Crippen Method |
| mcvol         | 186.400 | ml/mol  | McGowan Method |
| pc            | 2016.32 | kPa     | Joback Method  |
| tb            | 545.17  | K       | Joback Method  |
| tc            | 758.01  | K       | Joback Method  |
| tf            | 250.10  | K       | Joback Method  |
| vc            | 0.695   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 617.82    | J/mol×K | 758.01          | Joback Method |
| cpg           | 599.28    | J/mol×K | 722.54          | Joback Method |
| cpg           | 579.50    | J/mol×K | 687.06          | Joback Method |
| cpg           | 558.41    | J/mol×K | 651.59          | Joback Method |
| cpg           | 535.98    | J/mol×K | 616.12          | Joback Method |
| cpg           | 512.13    | J/mol×K | 580.64          | Joback Method |
| cpg           | 486.82    | J/mol×K | 545.17          | Joback Method |
| cpl           | 358.60    | J/mol×K | 313.00          | NIST Webbook  |
| dvisc         | 0.0004465 | Pa×s    | 495.99          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0005880 | Pa×s | 446.81 | Joback Method |
| dvisc | 0.0008290 | Pa×s | 397.63 | Joback Method |
| dvisc | 0.0012876 | Pa×s | 348.46 | Joback Method |
| dvisc | 0.0023113 | Pa×s | 299.28 | Joback Method |
| dvisc | 0.0052223 | Pa×s | 250.10 | Joback Method |
| dvisc | 0.0003563 | Pa×s | 545.17 | Joback Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C92369830&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92369830&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>                             |
| <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>cpl:</b>     | Liquid phase 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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