

# 1,4-Decadiyne

|                      |                                                          |
|----------------------|----------------------------------------------------------|
| Inchi:               | InChI=1S/C10H14/c1-3-5-7-9-10-8-6-4-2/h1H,4-6,8,10H2,2H3 |
| InchiKey:            | PITHRTPWTQFONM-UHFFFAOYSA-N                              |
| Formula:             | C10H14                                                   |
| SMILES:              | C#CCC#CCCCC                                              |
| Mol. weight [g/mol]: | 134.22                                                   |
| CAS:                 | 929-53-3                                                 |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 459.19  | kJ/mol  | Joback Method  |
| hf            | 314.47  | kJ/mol  | Joback Method  |
| hfus          | 27.75   | kJ/mol  | Joback Method  |
| hvap          | 39.86   | kJ/mol  | Joback Method  |
| log10ws       | -3.60   |         | Crippen Method |
| logp          | 2.593   |         | Crippen Method |
| mcvol         | 134.560 | ml/mol  | McGowan Method |
| pc            | 2859.68 | kPa     | Joback Method  |
| tb            | 427.32  | K       | Joback Method  |
| tc            | 625.25  | K       | Joback Method  |
| tf            | 355.53  | K       | Joback Method  |
| vc            | 0.519   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 259.37 | J/mol×K | 427.32          | Joback Method |
| cpg           | 272.43 | J/mol×K | 460.31          | Joback Method |
| cpg           | 284.89 | J/mol×K | 493.30          | Joback Method |
| cpg           | 296.76 | J/mol×K | 526.29          | Joback Method |
| cpg           | 308.07 | J/mol×K | 559.28          | Joback Method |
| cpg           | 318.84 | J/mol×K | 592.26          | Joback Method |
| cpg           | 329.09 | J/mol×K | 625.25          | Joback Method |

# Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 341.50 ± 0.50 | K    | 0.70           | NIST Webbook |
| tbrp          | 396.00 ± 1.00 | K    | 2.30           | NIST Webbook |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C929533&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C929533&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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