

# 1-Phenyl-1-(2-pyridyl)ethylene

|                      |                                                                     |
|----------------------|---------------------------------------------------------------------|
| Other names:         | Pyridine,2-(1-phenylethenyl)-<br>1-Phenyl-1-(2-pyridyl)ethylene     |
| Inchi:               | InChI=1S/C13H11N/c1-11(12-7-3-2-4-8-12)13-9-5-6-10-14-13/h2-10H,1H2 |
| InchiKey:            | WLFQFTSISRWCNV-UHFFFAOYSA-N                                         |
| Formula:             | C13H11N                                                             |
| SMILES:              | <chem>C=C(c1ccccc1)c1cccn1</chem>                                   |
| Mol. weight [g/mol]: | 181.24                                                              |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | 338.81  | kJ/mol | Cheméo Relay (1.0) |
| hvap          | 71.94   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 8.65    | eV     | NIST Webbook       |
| ie            | 8.65    | eV     | NIST Webbook       |
| log10ws       | -2.24   |        | Cheméo Relay (1.0) |
| logp          | 3.143   |        | Crippen Method     |
| mcvol         | 152.190 | ml/mol | McGowan Method     |
| tb            | 565.35  | K      | Cheméo Relay (1.0) |
| tf            | 293.80  | K      | Cheméo Relay (1.0) |

## Sources

|                           |                                                                                                                                               |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                     |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| Cheméo Relay (1.0):       |                                                                                                                                               |
| Cheméo Relay (1.0, beta): |                                                                                                                                               |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C15260658&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15260658&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hvac:</b>    | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>      | Ionization energy                               |
| <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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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