

# Diphenyl-1,2,5-oxadiazole

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Furazan, diphenyl-<br>3,4-Diphenyl-1,2,5-oxadiazole<br>3,4-Diphenylfurazan<br>Diphenylfurazan |
| <b>Inchi:</b>               | InChI=1S/C14H10N2O/c1-3-7-11(8-4-1)13-14(16-17-15-13)12-9-5-2-6-10-12/h1-10H                  |
| <b>InchiKey:</b>            | RIIIXRZGXAJVEQ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C14H10N2O   |
| <b>SMILES:</b>              | <chem>c1ccc(-c2nonc2-c2ccccc2)cc1</chem>  |
| <b>Mol. weight [g/mol]:</b> | 222.24  |
| <b>CAS:</b>                 | 19768-02-6  |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| chs           | -7267.20 ± 8.40 | kJ/mol | NIST Webbook   |
| log10ws       | -9.94           |        | Crippen Method |
| logp          | 3.404           |        | Crippen Method |
| mvol          | 166.970         | ml/mol | McGowan Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 475.20 | K    | 2.30           | NIST Webbook |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>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=C19768026&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19768026&amp;Units=SI</a> |

# Legend

|                 |                                       |
|-----------------|---------------------------------------|
| <b>chs:</b>     | Standard solid enthalpy of combustion |
| <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>tbrp:</b>    | Boiling point at reduced pressure     |

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