

# Benzene, (1-methyl-1-propenyl)-, (Z)-

|                      |                                                                                                                                                                                              |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-Butene, 2-phenyl-, (Z)-<br>(Z)-2-Phenyl-2-butene<br>trans-«alpha»,«beta»-Dimethylstilbene<br>trans-2-Phenyl-2-butene<br>2-Butene, 2-phenyl-, trans<br>trans-«alpha»,«beta»-Dimethylstyrene |
| Inchi:               | InChI=1S/C10H12/c1-3-9(2)10-7-5-4-6-8-10/h3-8H,1-2H3/b9-3-                                                                                                                                   |
| InchiKey:            | UGUYQBMBIJFNRM-OQFOIZHKSA-N                                                                                                                                                                  |
| Formula:             | C10H12                                                                                                                                                                                       |
| SMILES:              | CC=C(C)c1ccccc1                                                                                                                                                                              |
| Mol. weight [g/mol]: | 132.20                                                                                                                                                                                       |
| CAS:                 | 767-99-7                                                                                                                                                                                     |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 217.40        | kJ/mol  | Joback Method  |
| hf            | 94.23         | kJ/mol  | Joback Method  |
| hfus          | 14.59         | kJ/mol  | Joback Method  |
| hvap          | 40.17         | kJ/mol  | Joback Method  |
| log10ws       | -3.13         |         | Crippen Method |
| logp          | 3.110         |         | Crippen Method |
| mcvol         | 123.700       | ml/mol  | McGowan Method |
| pc            | 3121.00       | kPa     | Joback Method  |
| rinpol        | 1047.20       |         | NIST Webbook   |
| tb            | 446.15 ± 2.00 | K       | NIST Webbook   |
| tb            | 447.00 ± 2.50 | K       | NIST Webbook   |
| tc            | 678.24        | K       | Joback Method  |
| tf            | 209.84        | K       | Joback Method  |
| vc            | 0.469         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 240.06 | J/mol×K | 458.92          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 255.09 | J/mol×K | 495.47 | Joback Method |
| cpg | 269.14 | J/mol×K | 532.03 | Joback Method |
| cpg | 282.26 | J/mol×K | 568.58 | Joback Method |
| cpg | 294.51 | J/mol×K | 605.14 | Joback Method |
| cpg | 305.95 | J/mol×K | 641.69 | Joback Method |
| cpg | 316.62 | J/mol×K | 678.24 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C767997&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C767997&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>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>rinpola:</b> | Non-polar retention indices                     |
| <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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