

# Benzene, 1-ethenyl-3,5-dimethyl-

|                      |                                                                                                  |
|----------------------|--------------------------------------------------------------------------------------------------|
| Other names:         | 1,3-Dimethyl-5-vinylbenzene<br>3,5-Dimethylstyrene<br>5-Vinyl-m-xylene<br>Styrene, 3,5-dimethyl- |
| Inchi:               | InChI=1S/C10H12/c1-4-10-6-8(2)5-9(3)7-10/h4-7H,1H2,2-3H3                                         |
| InchiKey:            | XKMDZVINHIFHLY-UHFFFAOYSA-N                                                                      |
| Formula:             | C10H12                                                                                           |
| SMILES:              | C=Cc1cc(C)cc(C)c1                                                                                |
| Mol. weight [g/mol]: | 132.20                                                                                           |
| CAS:                 | 5379-20-4                                                                                        |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| gf            | 214.31        | kJ/mol  | Joback Method  |
| hf            | 89.29         | kJ/mol  | Joback Method  |
| hfus          | 13.64         | kJ/mol  | Joback Method  |
| hvap          | 40.78         | kJ/mol  | Joback Method  |
| log10ws       | -3.25         |         | Crippen Method |
| logp          | 2.946         |         | Crippen Method |
| mcvol         | 123.700       | ml/mol  | McGowan Method |
| pc            | 2969.80       | kPa     | Joback Method  |
| rinpol        | 1072.90       |         | NIST Webbook   |
| tb            | 461.52        | K       | Joback Method  |
| tc            | 673.43        | K       | Joback Method  |
| tf            | 212.96 ± 0.40 | K       | NIST Webbook   |
| vc            | 0.469         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 241.30 | J/mol×K | 461.52          | Joback Method |
| cpg           | 254.85 | J/mol×K | 496.84          | Joback Method |
| cpg           | 267.67 | J/mol×K | 532.16          | Joback Method |
| cpg           | 279.80 | J/mol×K | 567.47          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 291.26    | J/mol×K | 602.79 | Joback Method |
| cpg   | 302.08    | J/mol×K | 638.11 | Joback Method |
| cpg   | 312.28    | J/mol×K | 673.43 | Joback Method |
| dvisc | 0.0015433 | Pa×s    | 252.16 | Joback Method |
| dvisc | 0.0009004 | Pa×s    | 287.05 | Joback Method |
| dvisc | 0.0005904 | Pa×s    | 321.95 | Joback Method |
| dvisc | 0.0004204 | Pa×s    | 356.84 | Joback Method |
| dvisc | 0.0003181 | Pa×s    | 391.73 | Joback Method |
| dvisc | 0.0002519 | Pa×s    | 426.63 | Joback Method |
| dvisc | 0.0002066 | Pa×s    | 461.52 | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.45622e+01                   |
| Coeff. B                    | -3.89523e+03                  |
| Coeff. C                    | -7.05780e+01                  |
| Temperature range (K), min. | 343.46                        |
| Temperature range (K), max. | 491.65                        |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5379204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5379204&amp;Units=SI</a>                                             |
| The Yaws Handbook of Vapor Pressure: | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| Crippen Method:                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                                                               |
| 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>                                                                   |

## Legend

|        |                                         |
|--------|-----------------------------------------|
| cpg:   | Ideal gas heat capacity                 |
| dvisc: | Dynamic viscosity                       |
| gf:    | 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>pvap:</b>    | Vapor 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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