

Benzene, 1-ethenyl-4-fluoro-

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|-----------------------------|--------------------------------------------------------------------------------|
| Other names: | Styrene, p-fluoro- p-Fluorostyrene 4-Fluorostyrene para-Fluorostyrene |
| Inchi: | InChI=1S/C8H7F/c1-2-7-3-5-8(9)6-4-7/h2-6H,1H2 |
| InchiKey: | JWVTWJNGILGLAT-UHFFFAOYSA-N |
| Formula: | C8H7F |
| SMILES: | C=Cc1ccc(F)cc1 |
| Mol. weight [g/mol]: | 122.14 |
| CAS: | 405-99-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 12.29 | kJ/mol | Joback Method |
| hf | -54.07 | kJ/mol | Joback Method |
| hfus | 11.93 | kJ/mol | Joback Method |
| hvap | 34.85 | kJ/mol | Joback Method |
| log10ws | -2.63 | | Crippen Method |
| logp | 2.469 | | Crippen Method |
| mcvol | 97.290 | ml/mol | McGowan Method |
| pc | 3572.80 | kPa | Joback Method |
| rinpol | 904.00 | | NIST Webbook |
| rinpol | 904.00 | | NIST Webbook |
| rinpol | 894.00 | | NIST Webbook |
| tb | 410.05 | K | Joback Method |
| tc | 613.88 | K | Joback Method |
| tf | 217.69 | K | Joback Method |
| vc | 0.374 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 169.86 | J/molxK | 410.05 | Joback Method |
| cpg | 180.79 | J/molxK | 444.02 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 191.09 | J/mol×K | 477.99 | Joback Method |
| cpg | 200.80 | J/mol×K | 511.96 | Joback Method |
| cpg | 209.92 | J/mol×K | 545.94 | Joback Method |
| cpg | 218.50 | J/mol×K | 579.91 | Joback Method |
| cpg | 226.55 | J/mol×K | 613.88 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 340.60 | K | 6.70 | NIST Webbook |
| tbrp | 302.70 | K | 0.50 | NIST Webbook |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C405992&Units=SI |

Legend

| | |
|------------------|-------------------------------------------------|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpolar: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |

tf: Normal melting (fusion) point

vc: Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/73-248-6/Benzene-1-ethenyl-4-fluoro.pdf>

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