

# 1-Propene, 2-chloro-1,1,3,3,3-pentafluoro-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Propene, 2-chloropentafluoro-<br>2-Chloropentafluoro-1-propene<br>2-Chloropentafluoropropene |
| <b>Inchi:</b>               | InChI=1S/C3ClF5/c4-1(2(5)6)3(7,8)9   |
| <b>InchiKey:</b>            | YTCHAEAIYHLXBK-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C3ClF5   |
| <b>SMILES:</b>              | FC(F)=C(Cl)C(F)(F)F  |
| <b>Mol. weight [g/mol]:</b> | 166.48   |
| <b>CAS:</b>                 | 2804-50-4  |

## Physical Properties

| Property code | Value         | Unit                 | Source         |
|---------------|---------------|----------------------|----------------|
| gf            | -945.64       | kJ/mol               | Joback Method  |
| hf            | -1012.65      | kJ/mol               | Joback Method  |
| hfus          | 13.29         | kJ/mol               | Joback Method  |
| hvap          | 21.39         | kJ/mol               | Joback Method  |
| log10ws       | -2.94         |                      | Crippen Method |
| logp          | 2.896         |                      | Crippen Method |
| mcvol         | 69.920        | ml/mol               | McGowan Method |
| pc            | 3513.74       | kPa                  | Joback Method  |
| tb            | 280.00        | K                    | NIST Webbook   |
| tb            | 278.50 ± 0.50 | K                    | NIST Webbook   |
| tc            | 453.20        | K                    | Joback Method  |
| tf            | 125.86        | K                    | Joback Method  |
| vc            | 0.314         | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 115.95 | J/mol×K | 302.51          | Joback Method |
| cpg           | 121.95 | J/mol×K | 327.62          | Joback Method |
| cpg           | 127.54 | J/mol×K | 352.74          | Joback Method |
| cpg           | 132.75 | J/mol×K | 377.85          | Joback Method |
| cpg           | 137.58 | J/mol×K | 402.97          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 142.07 | J/mol×K | 428.08 | Joback Method |
| cpg | 146.22 | J/mol×K | 453.20 | Joback Method |

## 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>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>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2804504&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2804504&amp;Units=SI</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>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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