

1-Propyne, 1,3,3,3-tetrafluoro-

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|----------------------|---|
| Other names: | Perfluoro(methylacetylene) Propyne, tetrafluoro- Tetrafluoropropyne |
| Inchi: | InChI=1S/C3F4/c4-2-1-3(5,6)7 |
| InchiKey: | JOZGZOAPSZDKX-UHFFFAOYSA-N |
| Formula: | C3F4 |
| SMILES: | FC#CC(F)(F)F |
| Mol. weight [g/mol]: | 112.03 |
| CAS: | 20174-11-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -599.22 | kJ/mol | Joback Method |
| hf | -626.14 | kJ/mol | Joback Method |
| hfus | 11.55 | kJ/mol | Joback Method |
| hvap | 19.86 | kJ/mol | Joback Method |
| log10ws | -1.88 | | Crippen Method |
| logp | 1.479 | | Crippen Method |
| mcvol | 51.610 | ml/mol | McGowan Method |
| pc | 4403.25 | kPa | Joback Method |
| tb | 270.89 | K | Joback Method |
| tc | 427.18 | K | Joback Method |
| tf | 234.45 | K | Joback Method |
| vc | 0.227 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 103.27 | J/mol×K | 401.13 | Joback Method |
| cpg | 83.18 | J/mol×K | 270.89 | Joback Method |
| cpg | 87.72 | J/mol×K | 296.94 | Joback Method |
| cpg | 91.98 | J/mol×K | 322.99 | Joback Method |
| cpg | 95.99 | J/mol×K | 349.04 | Joback Method |
| cpg | 99.75 | J/mol×K | 375.08 | Joback Method |

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|-------|--------|---------|--------|---------------|
| cpg | 106.57 | J/mol×K | 427.18 | Joback Method |
| hvapt | 18.80 | kJ/mol | 198.50 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|--------------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{\text{vp}}) = A + B/(T + C)$ |
| Coeff. A | 1.47481e+01 |
| Coeff. B | -2.25653e+03 |
| Temperature range (K), min. | 156.05 |
| Temperature range (K), max. | 239.13 |

Sources

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|---|---|
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| 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=C20174112&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 |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| pvap: | Vapor pressure |

| | |
|------------|----------------------------------|
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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