

1,3-Pentadiyne, 1,5,5,5-tetrafluoro-

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|-----------------------------|----------------------------------|
| Other names: | 1,3-Pentadiyne, 5,5,5-trifluoro- |
| Inchi: | InChI=1S/C5F4/c6-4-2-1-3-5(7,8)9 |
| InchiKey: | MPUNIKDSZGUONG-UHFFFAOYSA-N |
| Formula: | C5F4 |
| SMILES: | FC#CC#CC(F)(F)F |
| Mol. weight [g/mol]: | 136.05 |
| CAS: | 64788-24-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -379.58 | kJ/mol | Joback Method |
| hf | -395.12 | kJ/mol | Joback Method |
| hfus | 19.86 | kJ/mol | Joback Method |
| hvap | 26.46 | kJ/mol | Joback Method |
| ie | 10.58 | eV | NIST Webbook |
| ie | 10.85 | eV | NIST Webbook |
| log10ws | -2.52 | | Crippen Method |
| logp | 1.482 | | Crippen Method |
| mcvol | 71.190 | ml/mol | McGowan Method |
| pc | 4222.04 | kPa | Joback Method |
| tb | 325.65 | K | Joback Method |
| tc | 510.79 | K | Joback Method |
| tf | 363.09 | K | Joback Method |
| vc | 0.300 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 119.56 | J/molxK | 325.65 | Joback Method |
| cpg | 125.17 | J/molxK | 356.51 | Joback Method |
| cpg | 130.41 | J/molxK | 387.36 | Joback Method |
| cpg | 135.30 | J/molxK | 418.22 | Joback Method |
| cpg | 139.86 | J/molxK | 449.08 | Joback Method |
| cpg | 144.09 | J/molxK | 479.94 | Joback Method |

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=C64788245&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 |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/75-887-5/1-3-Pentadiyne-1-5-5-5-tetrafluoro.pdf>

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