# Pentafluoropropionic acid, pentyl ester

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|---|---|
| **Other names:** | Pentyl pentafluoropropionate |
| | Pentyl 2,2,3,3,3-pentafluoropropanoate |
| | 1-Pentanol, pentafluoropropionate |
| | 2,2,3,3,3-Pentafluoro-propionic acid pentyl ester |
| | Pentyl pentafluoropropanoate |
| | Propanoic acid, pentafluoro, pentyl ester |
| **Inchi:** | InChI=1S/C8H11F5O2/c1-2-3-4-5-15-6(14)7(9,10)8(11,12)13/h2-5H2,1H3 |
| **InchiKey:** | BPYYNYLCDRAOKR-UHFFFAOYSA-N |
| **Formula:** | C8H11F5O2 |
| **SMILES:** | CCCCCOC(=O)C(F)(F)C(F)(F)F |
| **Mol. weight [g/mol]:** | 234.16 |
| **CAS:** | 680-29-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1185.81 | kJ/mol | Joback Method |
| hf | -1451.30 | kJ/mol | Joback Method |
| hfus | 19.84 | kJ/mol | Joback Method |
| hvap | 35.88 | kJ/mol | Joback Method |
| log10ws | -3.01 | | Crippen Method |
| logp | 2.917 | | Crippen Method |
| mcvol | 139.870 | ml/mol | McGowan Method |
| pc | 2210.37 | kPa | Joback Method |
| rinpol | 780.70 | | NIST Webbook |
| rinpol | 784.00 | | NIST Webbook |
| rinpol | 798.00 | | NIST Webbook |
| rinpol | 781.00 | | NIST Webbook |
| rinpol | 802.50 | | NIST Webbook |
| ripol | 820.00 | | NIST Webbook |
| tb | 448.62 | K | Joback Method |
| tc | 602.67 | K | Joback Method |
| tf | 259.87 | K | Joback Method |
| vc | 0.576 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 326.06 | J/mol×K | 448.62 | Joback Method |
| cpg | 337.69 | J/mol×K | 474.29 | Joback Method |
| cpg | 348.75 | J/mol×K | 499.97 | Joback Method |
| cpg | 359.26 | J/mol×K | 525.64 | Joback Method |
| cpg | 369.23 | J/mol×K | 551.32 | Joback Method |
| cpg | 378.69 | J/mol×K | 576.99 | Joback Method |
| cpg | 387.66 | J/mol×K | 602.67 | Joback Method |

# Sources

**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=C680295&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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
**rinpol:** Non-polar retention indices
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume