# Pentafluorobenzoic acid, benzyl ester

**Other names:** Benzyl 2,3,4,5,6-pentafluorobenzoate
Benzoic acid, pentafluoro-, phenylmethyl ester
Benzenemethanol, pentafluorobenzoate
**Inchi:** InChI=1S/C14H7F5O2/c15-9-8(10(16)12(18)13(19)11(9)17)14(20)21-6-7-4-2-1-3-5-7/h1-
**InchiKey:** WLPUFAZAMBXLPF-UHFFFAOYSA-N
**Formula:** C14H7F5O2
**SMILES:** O=C(OCc1ccccc1)c1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 302.20
**CAS:** 104856-46-4

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -964.30 | kJ/mol | Joback Method |
| hf | -1141.93 | kJ/mol | Joback Method |
| hfus | 36.34 | kJ/mol | Joback Method |
| hvap | 59.69 | kJ/mol | Joback Method |
| log10ws | -5.48 | | Crippen Method |
| logp | 3.739 | | Crippen Method |
| mcvol | 176.890 | ml/mol | McGowan Method |
| pc | 2155.30 | kPa | Joback Method |
| rinpol | 1583.00 | | NIST Webbook |
| rinpol | 1613.00 | | NIST Webbook |
| rinpol | 1613.00 | | NIST Webbook |
| rinpol | 1583.00 | | NIST Webbook |
| ripol | 2180.00 | | NIST Webbook |
| ripol | 2180.00 | | NIST Webbook |
| tb | 670.62 | K | Joback Method |
| tc | 868.93 | K | Joback Method |
| tf | 438.09 | K | Joback Method |
| vc | 0.718 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 450.93 | J/mol×K | 670.62 | Joback Method |
| cpg | 462.10 | J/mol×K | 703.67 | Joback Method |
| cpg | 472.57 | J/mol×K | 736.72 | Joback Method |
| cpg | 482.36 | J/mol×K | 769.77 | Joback Method |
| cpg | 491.46 | J/mol×K | 802.83 | Joback Method |
| cpg | 499.90 | J/mol×K | 835.88 | Joback Method |
| cpg | 507.68 | J/mol×K | 868.93 | Joback Method |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**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=C104856464&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
**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