# octyl pentafluorobenzoate

**Other names:** Benzoic acid, pentafluoro, octyl ester
**Inchi:** InChI=1S/C15H17F5O2/c1-2-3-4-5-6-7-8-22-15(21)9-10(16)12(18)14(20)13(19)11(9)17/h
**InchiKey:** KPGZPQWOOIGSIQ-UHFFFAOYSA-N
**Formula:** C15H17F5O2
**SMILES:** CCCCCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 324.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1068.29 | kJ/mol | Joback Method |
| hf | -1399.10 | kJ/mol | Joback Method |
| hfus | 44.89 | kJ/mol | Joback Method |
| hvap | 59.64 | kJ/mol | Joback Method |
| log10ws | -6.30 | | Crippen Method |
| logp | 4.899 | | Crippen Method |
| mcvol | 214.740 | ml/mol | McGowan Method |
| pc | 1501.15 | kPa | Joback Method |
| rinpol | 1615.00 | | NIST Webbook |
| rinpol | 1611.00 | | NIST Webbook |
| rinpol | 1611.00 | | NIST Webbook |
| rinpol | 1611.00 | | NIST Webbook |
| rinpol | 1620.00 | | NIST Webbook |
| rinpol | 1618.00 | | NIST Webbook |
| rinpol | 1615.00 | | NIST Webbook |
| rinpol | 1618.00 | | NIST Webbook |
| ripol | 1899.00 | | NIST Webbook |
| ripol | 1888.00 | | NIST Webbook |
| ripol | 1899.00 | | NIST Webbook |
| ripol | 1904.00 | | NIST Webbook |
| ripol | 1912.00 | | NIST Webbook |
| ripol | 1906.00 | | NIST Webbook |
| ripol | 1904.00 | | NIST Webbook |
| ripol | 1877.00 | | NIST Webbook |
| ripol | 1888.00 | | NIST Webbook |
| tb | 666.82 | K | Joback Method |
| tc | 836.45 | K | Joback Method |
| tf | 422.94 | K | Joback Method |

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|---|---|---|---|
| vc | 0.881 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 584.22 | J/mol×K | 666.82 | Joback Method |
| cpg | 597.38 | J/mol×K | 695.09 | Joback Method |
| cpg | 609.94 | J/mol×K | 723.36 | Joback Method |
| cpg | 621.91 | J/mol×K | 751.63 | Joback Method |
| cpg | 633.29 | J/mol×K | 779.90 | Joback Method |
| cpg | 644.10 | J/mol×K | 808.18 | Joback Method |
| cpg | 654.32 | J/mol×K | 836.45 | Joback Method |

# Sources

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|---|---|
| **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=R35143&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 |