# Isobutyric acid, 2,3,4,6-tetrachlorophenyl ester

**Inchi:** InChI=1S/C10H8Cl4O2/c1-4(2)10(15)16-9-6(12)3-5(11)7(13)8(9)14/h3-4H,1-2H3
**InchiKey:** VBLZPANJGHZOMW-UHFFFAOYSA-N
**Formula:** C10H8Cl4O2
**SMILES:** CC(C)C(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
**Mol. weight [g/mol]:** 301.98

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -176.87 | kJ/mol | Joback Method |
| hf | -372.12 | kJ/mol | Joback Method |
| hfus | 30.19 | kJ/mol | Joback Method |
| hvap | 69.09 | kJ/mol | Joback Method |
| log10ws | -5.12 | | Crippen Method |
| logp | 4.862 | | Crippen Method |
| mcvol | 184.400 | ml/mol | McGowan Method |
| pc | 2497.50 | kPa | Joback Method |
| rinpol | 1833.00 | | NIST Webbook |
| rinpol | 1833.00 | | NIST Webbook |
| tb | 700.37 | K | Joback Method |
| tc | 935.73 | K | Joback Method |
| tf | 455.80 | K | Joback Method |
| vc | 0.702 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 390.16 | J/mol×K | 700.37 | Joback Method |
| cpg | 399.73 | J/mol×K | 739.60 | Joback Method |
| cpg | 408.61 | J/mol×K | 778.82 | Joback Method |
| cpg | 416.79 | J/mol×K | 818.05 | Joback Method |
| cpg | 424.27 | J/mol×K | 857.28 | Joback Method |
| cpg | 431.07 | J/mol×K | 896.50 | Joback Method |
| cpg | 437.17 | J/mol×K | 935.73 | Joback Method |
| dvisc | 0.0008154 | Pa×s | 455.80 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0005515 | Pa×s | 496.56 | Joback Method |
| dvisc | 0.0003957 | Pa×s | 537.32 | Joback Method |
| dvisc | 0.0002976 | Pa×s | 578.09 | Joback Method |
| dvisc | 0.0002324 | Pa×s | 618.85 | Joback Method |
| dvisc | 0.0001871 | Pa×s | 659.61 | Joback Method |
| dvisc | 0.0001544 | Pa×s | 700.37 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354641&Units=SI |
| **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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |