# 1,2-Cyclohexanedicarboxylic acid, isobutyl 2,4,6-trichlorophenyl ester

**Inchi:** InChI=1S/C18H21Cl3O4/c1-10(2)9-24-17(22)12-5-3-4-6-13(12)18(23)25-16-14(20)7-11(

**InchiKey:** JWLXFBMPAPOBSF-UHFFFAOYSA-N

**Formula:** C18H21Cl3O4

**SMILES:** CC(C)COC(=O)C1CCCCC1C(=O)Oc1c(Cl)cc(Cl)cc1Cl

**Mol. weight [g/mol]:** 407.72

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -305.13 | kJ/mol | Joback Method |
| hf | -720.85 | kJ/mol | Joback Method |
| hfus | 42.80 | kJ/mol | Joback Method |
| hvap | 91.12 | kJ/mol | Joback Method |
| log10ws | -6.06 | | Crippen Method |
| logp | 5.558 | | Crippen Method |
| mcvol | 281.460 | ml/mol | McGowan Method |
| pc | 1601.28 | kPa | Joback Method |
| rinpol | 2637.00 | | NIST Webbook |
| rinpol | 2637.00 | | NIST Webbook |
| tb | 932.17 | K | Joback Method |
| tc | 1169.25 | K | Joback Method |
| tf | 578.82 | K | Joback Method |
| vc | 1.056 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 832.03 | J/mol×K | 932.17 | Joback Method |
| cpg | 878.35 | J/mol×K | 1129.74 | Joback Method |
| cpg | 872.27 | J/mol×K | 1090.23 | Joback Method |
| cpg | 864.60 | J/mol×K | 1050.71 | Joback Method |
| cpg | 855.35 | J/mol×K | 1011.20 | Joback Method |
| cpg | 844.50 | J/mol×K | 971.68 | Joback Method |
| cpg | 882.88 | J/mol×K | 1169.25 | Joback Method |
| dvisc | 0.0000595 | Pa×s | 932.17 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000742 | Pa×s | 873.28 | Joback Method |
| dvisc | 0.0000955 | Pa×s | 814.39 | Joback Method |
| dvisc | 0.0001279 | Pa×s | 755.50 | Joback Method |
| dvisc | 0.0001799 | Pa×s | 696.60 | Joback Method |
| dvisc | 0.0002695 | Pa×s | 637.71 | Joback Method |
| dvisc | 0.0004384 | Pa×s | 578.82 | 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=U339807&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |