# Isophthalic acid, 3,4-dimethylcyclohexyl isobutyl ester

**Inchi:** InChI=1S/C20H28O4/c1-13(2)12-23-19(21)16-6-5-7-17(11-16)20(22)24-18-9-8-14(3)15(4

**InchiKey:** SQABXCZHPURDHQ-UHFFFAOYSA-N

**Formula:** C20H28O4

**SMILES:** CC(C)COC(=O)c1cccc(C(=O)OC2CCC(C)C(C)C2)c1

**Mol. weight [g/mol]:** 332.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -240.95 | kJ/mol | Joback Method |
| hf | -712.31 | kJ/mol | Joback Method |
| hfus | 37.24 | kJ/mol | Joback Method |
| hvap | 80.79 | kJ/mol | Joback Method |
| log10ws | -5.42 | | Crippen Method |
| logp | 4.481 | | Crippen Method |
| mcvol | 272.920 | ml/mol | McGowan Method |
| pc | 1498.83 | kPa | Joback Method |
| rinpol | 2530.00 | | NIST Webbook |
| tb | 851.01 | K | Joback Method |
| tc | 1072.70 | K | Joback Method |
| tf | 482.32 | K | Joback Method |
| vc | 1.020 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 881.13 | J/mol×K | 851.01 | Joback Method |
| cpg | 899.09 | J/mol×K | 887.96 | Joback Method |
| cpg | 915.40 | J/mol×K | 924.91 | Joback Method |
| cpg | 930.08 | J/mol×K | 961.85 | Joback Method |
| cpg | 943.15 | J/mol×K | 998.80 | Joback Method |
| cpg | 954.63 | J/mol×K | 1035.75 | Joback Method |
| cpg | 964.51 | J/mol×K | 1072.70 | Joback Method |
| dvisc | 0.0008820 | Pa×s | 482.32 | Joback Method |
| dvisc | 0.0004820 | Pa×s | 543.77 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002978 | Pa×s | 605.22 | Joback Method |
| dvisc | 0.0002011 | Pa×s | 666.66 | Joback Method |
| dvisc | 0.0001451 | Pa×s | 728.11 | Joback Method |
| dvisc | 0.0001101 | Pa×s | 789.56 | Joback Method |
| dvisc | 0.0000870 | Pa×s | 851.01 | 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=U343802&Units=SI

# 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