# Bis(3-methylbutan-2-yl) phthalate

**Other names:** 1,2-Benzenedicarboxylic acid, bis(3-methylbutan-2-yl) ester
Bis(3-methylbutan-2-yl)-1,2-benzenedicarboxylate
**Inchi:** InChI=1S/C18H26O4/c1-11(2)13(5)21-17(19)15-9-7-8-10-16(15)18(20)22-14(6)12(3)4/h7
**InchiKey:** KYBCYUKYPGQBSB-UHFFFAOYSA-N
**Formula:** C18H26O4
**SMILES:** CC(C)C(C)OC(=O)c1ccccc1C(=O)OC(C)C(C)C
**Mol. weight [g/mol]:** 306.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -274.14 | kJ/mol | Joback Method |
| hf | -700.51 | kJ/mol | Joback Method |
| hfus | 27.51 | kJ/mol | Joback Method |
| hvap | 75.36 | kJ/mol | Joback Method |
| log10ws | -5.05 | | Crippen Method |
| logp | 4.089 | | Crippen Method |
| mcvol | 255.600 | ml/mol | McGowan Method |
| pc | 1592.35 | kPa | Joback Method |
| rinpol | 1991.00 | | NIST Webbook |
| rinpol | 1991.00 | | NIST Webbook |
| tb | 793.72 | K | Joback Method |
| tc | 1003.71 | K | Joback Method |
| tf | 415.88 | K | Joback Method |
| vc | 0.960 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 763.39 | J/mol×K | 793.72 | Joback Method |
| cpg | 779.87 | J/mol×K | 828.72 | Joback Method |
| cpg | 795.15 | J/mol×K | 863.72 | Joback Method |
| cpg | 809.25 | J/mol×K | 898.71 | Joback Method |
| cpg | 822.19 | J/mol×K | 933.71 | Joback Method |
| cpg | 833.99 | J/mol×K | 968.71 | Joback Method |

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|---|---|---|---|---|
| cpg | 844.67 | J/mol×K | 1003.71 | Joback Method |
| dvisc | 0.0013805 | Pa×s | 415.88 | Joback Method |
| dvisc | 0.0005561 | Pa×s | 478.85 | Joback Method |
| dvisc | 0.0002768 | Pa×s | 541.83 | Joback Method |
| dvisc | 0.0001593 | Pa×s | 604.80 | Joback Method |
| dvisc | 0.0001017 | Pa×s | 667.77 | Joback Method |
| dvisc | 0.0000702 | Pa×s | 730.75 | Joback Method |
| dvisc | 0.0000514 | Pa×s | 793.72 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U373656&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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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

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