# (E)-3-Butylidene phthalide

**Other names:** 3-Butylidenephthalide, (E)-
**Inchi:** InChI=1S/C12H12O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h4-8H,2-3H2,1H3/b11-8+
**InchiKey:** WMBOCUXXNSOQHM-DHZHZOJOSA-N
**Formula:** C12H12O2
**SMILES:** CCCC=C1OC(=O)c2ccccc21
**Mol. weight [g/mol]:** 188.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 58.15 | kJ/mol | Joback Method |
| hf | -166.48 | kJ/mol | Joback Method |
| hfus | 25.36 | kJ/mol | Joback Method |
| hvap | 55.01 | kJ/mol | Joback Method |
| log10ws | -3.76 | | Crippen Method |
| logp | 2.998 | | Crippen Method |
| mcvol | 148.460 | ml/mol | McGowan Method |
| pc | 2966.57 | kPa | Joback Method |
| rinpol | 1722.00 | | NIST Webbook |
| rinpol | 1722.00 | | NIST Webbook |
| rinpol | 1707.00 | | NIST Webbook |
| rinpol | 1707.00 | | NIST Webbook |
| rinpol | 1677.00 | | NIST Webbook |
| ripol | 2554.00 | | NIST Webbook |
| ripol | 2554.00 | | NIST Webbook |
| tb | 618.44 | K | Joback Method |
| tc | 853.60 | K | Joback Method |
| tf | 391.27 | K | Joback Method |
| vc | 0.569 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 369.95 | J/mol×K | 618.44 | Joback Method |
| cpg | 384.23 | J/mol×K | 657.63 | Joback Method |

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|---|---|---|---|---|
| cpg | 397.57 | J/mol×K | 696.83 | Joback Method |
| cpg | 410.03 | J/mol×K | 736.02 | Joback Method |
| cpg | 421.65 | J/mol×K | 775.21 | Joback Method |
| cpg | 432.48 | J/mol×K | 814.40 | Joback Method |
| cpg | 442.57 | J/mol×K | 853.60 | 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=R87754&Units=SI |

# Legend

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