

# 1(3H)-Isobenzofuranone, 3-butylidene-

<b>Other names:</b>	BdPh Butylidenephthalide Phthalide, 3-butylidene- 3-Butylidenephthalide n-Butylidene phthalide
<b>Inchi:</b>	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-
<b>InchiKey:</b>	WMBOCUXXNSOQHM-FLIBITNWSA-N
<b>Formula:</b>	C12H12O2
<b>SMILES:</b>	CCCC=C1OC(=O)c2ccccc21
<b>Mol. weight [g/mol]:</b>	188.22
<b>CAS:</b>	551-08-6

## 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	1678.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1670.00		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
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

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C551086&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C551086&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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