

# 3-(Butyl(2-[butyl(3-oxo-1,3-dihydro-2-benzofuran-

<b>Inchi:</b>	InChI=1S/C26H32N2O4/c1-3-5-15-27(23-19-11-7-9-13-21(19)25(29)31-23)17-18-28(16-
<b>InchiKey:</b>	KWTXMBJOCBWQBY-UHFFFAOYSA-N
<b>Formula:</b>	C26H32N2O4
<b>SMILES:</b>	CCCCN(CCN(CCCC)C1OC(=O)c2ccccc21)C1OC(=O)c2ccccc21
<b>Mol. weight [g/mol]:</b>	436.54

## Physical Properties

Property code	Value	Unit	Source
gf	299.24	kJ/mol	Joback Method
hf	-388.59	kJ/mol	Joback Method
hfus	67.69	kJ/mol	Joback Method
hvap	100.77	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	4.929		Crippen Method
mcvol	342.800	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
tb	1085.50	K	Joback Method
tc	1332.36	K	Joback Method
tf	751.06	K	Joback Method
vc	1.282	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.98	J/molxK	1085.50	Joback Method
cpg	1240.96	J/molxK	1126.64	Joback Method
cpg	1254.74	J/molxK	1167.79	Joback Method
cpg	1267.45	J/molxK	1208.93	Joback Method
cpg	1279.23	J/molxK	1250.08	Joback Method
cpg	1290.23	J/molxK	1291.22	Joback Method
cpg	1300.57	J/molxK	1332.36	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=B6001130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001130&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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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