

# 3-(Beta-methoxyethyl)-3-phenyl-2-benzofuranone

<b>Inchi:</b>	InChI=1S/C17H16O3/c1-19-12-11-17(13-7-3-2-4-8-13)14-9-5-6-10-15(14)20-16(17)18/h2
<b>InchiKey:</b>	RJWYAYIWXFJXBK-UHFFFAOYSA-N
<b>Formula:</b>	C17H16O3
<b>SMILES:</b>	COCCC1(c2ccccc2)C(=O)Oc2ccccc21
<b>Mol. weight [g/mol]:</b>	268.31
<b>CAS:</b>	95279-90-6

## Physical Properties

Property code	Value	Unit	Source
gf	49.00	kJ/mol	Joback Method
hf	-246.50	kJ/mol	Joback Method
hfus	27.99	kJ/mol	Joback Method
hvap	68.58	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.928		Crippen Method
mvol	205.320	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	770.87	K	Joback Method
tc	1025.18	K	Joback Method
tf	505.57	K	Joback Method
vc	0.772	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.76	J/molxK	770.87	Joback Method
cpg	610.98	J/molxK	813.26	Joback Method
cpg	627.44	J/molxK	855.64	Joback Method
cpg	643.34	J/molxK	898.03	Joback Method
cpg	658.88	J/molxK	940.41	Joback Method
cpg	674.26	J/molxK	982.80	Joback Method
cpg	689.68	J/molxK	1025.18	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=C95279906&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C95279906&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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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