

# 3-Phenyl-6-benzoyl-alpha-pyrone

<b>Inchi:</b>	InChI=1S/C18H12O3/c19-17(14-9-5-2-6-10-14)16-12-11-15(18(20)21-16)13-7-3-1-4-8-13
<b>InchiKey:</b>	WZZSWNVLVXGHDV-UHFFFAOYSA-N
<b>Formula:</b>	C18H12O3
<b>SMILES:</b>	O=C(c1ccccc1)c1ccc(-c2ccccc2)c(=O)o1
<b>Mol. weight [g/mol]:</b>	276.29
<b>CAS:</b>	116659-67-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.19		Crippen Method
logp	3.538		Crippen Method
mcvol	206.510	ml/mol	McGowan Method

## Sources

<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=C116659677&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659677&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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