

# Succinic acid, but-3-yn-2-yl 4-biphenyl ester

**Inchi:** InChI=1S/C20H18O4/c1-3-15(2)23-19(21)13-14-20(22)24-18-11-9-17(10-12-18)16-7-5-4  
**InchiKey:** QPEGSWSGEGASGCR-UHFFFAOYSA-N  
**Formula:** C20H18O4  
**SMILES:** C#CC(C)OC(=O)CCC(=O)Oc1ccc(-c2ccccc2)cc1  
**Mol. weight [g/mol]:** 322.35

## Physical Properties

Property code	Value	Unit	Source
gf	85.50	kJ/mol	Joback Method
hf	-197.52	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	83.11	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	3.604		Crippen Method
mvol	251.420	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	857.60	K	Joback Method
tc	1094.93	K	Joback Method
tf	556.81	K	Joback Method
vc	0.944	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.88	J/mol×K	857.60	Joback Method
cpg	739.49	J/mol×K	897.16	Joback Method
cpg	751.81	J/mol×K	936.71	Joback Method
cpg	762.88	J/mol×K	976.27	Joback Method
cpg	772.77	J/mol×K	1015.82	Joback Method
cpg	781.51	J/mol×K	1055.38	Joback Method
cpg	789.18	J/mol×K	1094.93	Joback Method

# Sources

<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>
<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=U390081&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390081&amp;Units=SI</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>rinpola:</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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