

# Sebacic acid, butyl but-3-yn-2-yl ester

**Inchi:** InChI=1S/C18H30O4/c1-4-6-15-21-17(19)13-11-9-7-8-10-12-14-18(20)22-16(3)5-2/h2,16  
**InchiKey:** CJHIQMFDDLJXHJ-UHFFFAOYSA-N  
**Formula:** C18H30O4  
**SMILES:** C#CC(C)OC(=O)CCCCCCCCC(=O)OCCCC  
**Mol. weight [g/mol]:** 310.43

## Physical Properties

Property code	Value	Unit	Source
gf	-146.53	kJ/mol	Joback Method
hf	-617.83	kJ/mol	Joback Method
hfus	47.40	kJ/mol	Joback Method
hvap	73.44	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.015		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpola	2107.00		NIST Webbook
rinpola	2107.00		NIST Webbook
tb	753.50	K	Joback Method
tc	937.87	K	Joback Method
tf	468.91	K	Joback Method
vc	1.048	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.18	J/molxK	753.50	Joback Method
cpg	813.77	J/molxK	784.23	Joback Method
cpg	829.46	J/molxK	814.96	Joback Method
cpg	844.27	J/molxK	845.68	Joback Method
cpg	858.21	J/molxK	876.41	Joback Method
cpg	871.30	J/molxK	907.14	Joback Method
cpg	883.56	J/molxK	937.87	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=U355845&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355845&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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