

# Succinic acid, butyl 3-methylbenzyl ester

**Inchi:** InChI=1S/C16H22O4/c1-3-4-10-19-15(17)8-9-16(18)20-12-14-7-5-6-13(2)11-14/h5-7,11H  
**InchiKey:** OIYVHXRJPIPRRC-UHFFFAOYSA-N  
**Formula:** C16H22O4  
**SMILES:** CCCOC(=O)CCC(=O)OCc1cccc(C)c1  
**Mol. weight [g/mol]:** 278.34

## Physical Properties

Property code	Value	Unit	Source
gf	-281.22	kJ/mol	Joback Method
hf	-638.11	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.162		Crippen Method
mvol	227.420	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	749.72	K	Joback Method
tc	951.49	K	Joback Method
tf	453.34	K	Joback Method
vc	0.872	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.45	J/molxK	749.72	Joback Method
cpg	714.48	J/molxK	917.86	Joback Method
cpg	703.17	J/molxK	884.24	Joback Method
cpg	690.92	J/molxK	850.61	Joback Method
cpg	677.73	J/molxK	816.98	Joback Method
cpg	663.58	J/molxK	783.35	Joback Method
cpg	724.87	J/molxK	951.49	Joback Method
dvisc	0.0000934	Paxs	749.72	Joback Method

dvisc	0.0001185	Paxs	700.32	Joback Method
dvisc	0.0001560	Paxs	650.93	Joback Method
dvisc	0.0002148	Paxs	601.53	Joback Method
dvisc	0.0003132	Paxs	552.13	Joback Method
dvisc	0.0004919	Paxs	502.74	Joback Method
dvisc	0.0008522	Paxs	453.34	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=U382391&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382391&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>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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