

# Succinic acid, 5-bromo-2-methoxybenzyl nonyl ester

**Inchi:** InChI=1S/C21H31BrO5/c1-3-4-5-6-7-8-9-14-26-20(23)12-13-21(24)27-16-17-15-18(22)1  
**InchiKey:** HYKJYYWMQGCZDX-UHFFFAOYSA-N  
**Formula:** C21H31BrO5  
**SMILES:** CCCCCCCCCOC(=O)CCC(=O)OCc1cc(Br)ccc1OC  
**Mol. weight [g/mol]:** 443.37

## Physical Properties

Property code	Value	Unit	Source
gf	-339.43	kJ/mol	Joback Method
hf	-858.67	kJ/mol	Joback Method
hfus	55.46	kJ/mol	Joback Method
hvap	93.10	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.575		Crippen Method
mvol	321.240	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2949.00		NIST Webbook
rinpol	2949.00		NIST Webbook
tb	957.68	K	Joback Method
tc	1174.68	K	Joback Method
tf	604.24	K	Joback Method
vc	1.232	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.65	J/molxK	957.68	Joback Method
cpg	1018.52	J/molxK	993.85	Joback Method
cpg	1031.03	J/molxK	1030.01	Joback Method
cpg	1042.19	J/molxK	1066.18	Joback Method
cpg	1052.04	J/molxK	1102.35	Joback Method
cpg	1060.58	J/molxK	1138.51	Joback Method
cpg	1067.83	J/molxK	1174.68	Joback Method
dvisc	0.0002168	Paxs	604.24	Joback Method

dvisc	0.0001323	Paxs	663.15	Joback Method
dvisc	0.0000875	Paxs	722.05	Joback Method
dvisc	0.0000616	Paxs	780.96	Joback Method
dvisc	0.0000455	Paxs	839.87	Joback Method
dvisc	0.0000350	Paxs	898.77	Joback Method
dvisc	0.0000278	Paxs	957.68	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=U381078&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381078&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>

## 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>mccvol:</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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