

# Succinic acid, 2-bromobenzyl nonyl ester

**Inchi:** InChI=1S/C20H29BrO4/c1-2-3-4-5-6-7-10-15-24-19(22)13-14-20(23)25-16-17-11-8-9-12  
**InchiKey:** KFYATYJUOAGNQW-UHFFFAOYSA-N  
**Formula:** C20H29BrO4  
**SMILES:** CCCCCCCCCOC(=O)CCC(=O)OCc1ccccc1Br  
**Mol. weight [g/mol]:** 413.35

## Physical Properties

Property code	Value	Unit	Source
gf	-233.22	kJ/mol	Joback Method
hf	-694.34	kJ/mol	Joback Method
hfus	52.07	kJ/mol	Joback Method
hvap	87.80	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.566		Crippen Method
mvol	301.280	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2732.00		NIST Webbook
rinpol	2732.00		NIST Webbook
tb	907.40	K	Joback Method
tc	1118.87	K	Joback Method
tf	558.22	K	Joback Method
vc	1.157	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.16	J/molxK	907.40	Joback Method
cpg	932.61	J/molxK	942.64	Joback Method
cpg	945.91	J/molxK	977.89	Joback Method
cpg	958.11	J/molxK	1013.13	Joback Method
cpg	969.22	J/molxK	1048.38	Joback Method
cpg	979.30	J/molxK	1083.62	Joback Method
cpg	988.36	J/molxK	1118.87	Joback Method
dvisc	0.0003888	Paxs	558.22	Joback Method

dvisc	0.0002264	Paxs	616.42	Joback Method
dvisc	0.0001448	Paxs	674.61	Joback Method
dvisc	0.0000994	Paxs	732.81	Joback Method
dvisc	0.0000721	Paxs	791.01	Joback Method
dvisc	0.0000546	Paxs	849.20	Joback Method
dvisc	0.0000429	Paxs	907.40	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=U381123&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381123&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>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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