

# Succinic acid, 1-(3-bromophenyl)ethyl nonyl ester

Inchi:	InChI=1S/C21H31BrO4/c1-3-4-5-6-7-8-9-15-25-20(23)13-14-21(24)26-17(2)18-11-10-12
InchiKey:	XOBKVZHQVXXWLF-UHFFFAOYSA-N
Formula:	C21H31BrO4
SMILES:	CCCCCCCCCOC(=O)CCC(=O)OC(C)c1cccc(Br)c1
Mol. weight [g/mol]:	427.37

## Physical Properties

Property code	Value	Unit	Source
gf	-227.24	kJ/mol	Joback Method
hf	-720.26	kJ/mol	Joback Method
hfus	51.13	kJ/mol	Joback Method
hvap	89.64	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.127		Crippen Method
mvol	315.370	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	929.84	K	Joback Method
tc	1144.23	K	Joback Method
tf	554.49	K	Joback Method
vc	1.208	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.10	J/molxK	929.84	Joback Method
cpg	992.81	J/molxK	965.57	Joback Method
cpg	1006.29	J/molxK	1001.30	Joback Method
cpg	1018.60	J/molxK	1037.04	Joback Method
cpg	1029.76	J/molxK	1072.77	Joback Method
cpg	1039.83	J/molxK	1108.50	Joback Method
cpg	1048.83	J/molxK	1144.23	Joback Method
dvisc	0.0003800	Paxs	554.49	Joback Method

dvisc	0.0002067	Paxs	617.05	Joback Method
dvisc	0.0001258	Paxs	679.61	Joback Method
dvisc	0.0000833	Paxs	742.16	Joback Method
dvisc	0.0000587	Paxs	804.72	Joback Method
dvisc	0.0000436	Paxs	867.28	Joback Method
dvisc	0.0000337	Paxs	929.84	Joback Method

## Sources

<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=U381470&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381470&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>
<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>

## 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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