

# Succinic acid, 8-chlorooctyl 3-phenylpropyl ester

Inchi:	InChI=1S/C21H31ClO4/c22-16-8-3-1-2-4-9-17-25-20(23)14-15-21(24)26-18-10-13-19-11
InchiKey:	SPNVQXLVPWTNGX-UHFFFAOYSA-N
Formula:	C21H31ClO4
SMILES:	O=C(CCC(=O)OCCc1ccccc1)OCCCCCCCCl
Mol. weight [g/mol]:	382.92

## Physical Properties

Property code	Value	Unit	Source
gf	-241.42	kJ/mol	Joback Method
hf	-745.58	kJ/mol	Joback Method
hfus	53.96	kJ/mol	Joback Method
hvap	87.31	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.065		Crippen Method
mvol	310.110	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tb	896.57	K	Joback Method
tc	1102.74	K	Joback Method
tf	527.09	K	Joback Method
vc	1.200	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.13	J/molxK	896.57	Joback Method
cpg	980.40	J/molxK	930.93	Joback Method
cpg	994.48	J/molxK	965.29	Joback Method
cpg	1007.40	J/molxK	999.66	Joback Method
cpg	1019.20	J/molxK	1034.02	Joback Method
cpg	1029.92	J/molxK	1068.38	Joback Method
cpg	1039.59	J/molxK	1102.74	Joback Method
dvisc	0.0005010	Paxs	527.09	Joback Method

dvisc	0.0002640	Paxs	588.67	Joback Method
dvisc	0.0001570	Paxs	650.25	Joback Method
dvisc	0.0001022	Paxs	711.83	Joback Method
dvisc	0.0000712	Paxs	773.41	Joback Method
dvisc	0.0000523	Paxs	834.99	Joback Method
dvisc	0.0000401	Paxs	896.57	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=U389735&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389735&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>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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