

# Sebacic acid, 8-chlorooctyl nonyl ester

**Inchi:** InChI=1S/C27H51ClO4/c1-2-3-4-5-9-14-19-24-31-26(29)21-16-11-6-7-12-17-22-27(30)32  
**InchiKey:** IRCLOFLNAPXQCY-UHFFFAOYSA-N  
**Formula:** C27H51ClO4  
**SMILES:** CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCI  
**Mol. weight [g/mol]:** 475.14

## Physical Properties

Property code	Value	Unit	Source
gf	-303.31	kJ/mol	Joback Method
hf	-1105.95	kJ/mol	Joback Method
hfus	75.46	kJ/mol	Joback Method
hvap	98.39	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	8.524		Crippen Method
mcvol	418.410	ml/mol	McGowan Method
pc	709.22	kPa	Joback Method
rinpol	3405.00		NIST Webbook
rinpol	3405.00		NIST Webbook
tb	1007.17	K	Joback Method
tc	1250.03	K	Joback Method
tf	568.29	K	Joback Method
vc	1.645	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.54	J/molxK	1007.17	Joback Method
cpg	1526.02	J/molxK	1209.55	Joback Method
cpg	1512.38	J/molxK	1169.08	Joback Method
cpg	1496.99	J/molxK	1128.60	Joback Method
cpg	1479.77	J/molxK	1088.12	Joback Method
cpg	1460.65	J/molxK	1047.65	Joback Method
cpg	1537.98	J/molxK	1250.03	Joback Method
dvisc	0.0000153	Paxs	1007.17	Joback Method

dvisc	0.0000205	Paxs	934.02	Joback Method
dvisc	0.0000289	Paxs	860.88	Joback Method
dvisc	0.0000434	Paxs	787.73	Joback Method
dvisc	0.0000707	Paxs	714.58	Joback Method
dvisc	0.0001289	Paxs	641.44	Joback Method
dvisc	0.0002741	Paxs	568.29	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=U355536&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355536&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>
<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>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10ws</sub>:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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