

# Sebacic acid, dodecyl nonyl ester

<b>Inchi:</b>	InChI=1S/C31H60O4/c1-3-5-7-9-11-12-13-17-21-25-29-35-31(33)27-23-19-15-14-18-22-
<b>InchiKey:</b>	YVFVPHMILPRZLE-UHFFFAOYSA-N
<b>Formula:</b>	C31H60O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	496.81

## Physical Properties

Property code	Value	Unit	Source
gf	-257.70	kJ/mol	Joback Method
hf	-1172.77	kJ/mol	Joback Method
hfus	81.62	kJ/mol	Joback Method
hvap	102.91	kJ/mol	Joback Method
log10ws	-10.52		Crippen Method
logp	9.865		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	594.30	kPa	Joback Method
rinsol	3542.00		NIST Webbook
tb	1061.26	K	Joback Method
tc	1344.42	K	Joback Method
tf	583.45	K	Joback Method
vc	1.819	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.89	J/molxK	1061.26	Joback Method
cpg	1696.10	J/molxK	1108.45	Joback Method
cpg	1718.46	J/molxK	1155.65	Joback Method
cpg	1738.13	J/molxK	1202.84	Joback Method
cpg	1755.25	J/molxK	1250.03	Joback Method
cpg	1769.95	J/molxK	1297.22	Joback Method
cpg	1782.40	J/molxK	1344.42	Joback Method
dvisc	0.0002077	Paxs	583.45	Joback Method
dvisc	0.0000918	Paxs	663.08	Joback Method

dvisc	0.0000484	Paxs	742.72	Joback Method
dvisc	0.0000288	Paxs	822.36	Joback Method
dvisc	0.0000188	Paxs	901.99	Joback Method
dvisc	0.0000132	Paxs	981.62	Joback Method
dvisc	0.0000097	Paxs	1061.26	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354269&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354269&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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