

# Sebacic acid, 3-methylphenyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C30H50O4/c1-3-4-5-6-7-8-9-10-13-16-19-25-33-29(31)23-17-14-11-12-15-18-2
<b>InchiKey:</b>	UEPPWVODQUMDON-UHFFFAOYSA-N
<b>Formula:</b>	C30H50O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	474.72

## Physical Properties

Property code	Value	Unit	Source
gf	-163.34	kJ/mol	Joback Method
hf	-927.07	kJ/mol	Joback Method
hfus	72.68	kJ/mol	Joback Method
hvap	103.62	kJ/mol	Joback Method
log10ws	-9.91		Crippen Method
logp	8.875		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	734.42	kPa	Joback Method
rinpola	3603.00		NIST Webbook
tb	1070.04	K	Joback Method
tc	1324.57	K	Joback Method
tf	611.12	K	Joback Method
vc	1.655	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1496.84	J/molxK	1070.04	Joback Method
cpg	1515.88	J/molxK	1112.46	Joback Method
cpg	1532.83	J/molxK	1154.88	Joback Method
cpg	1547.78	J/molxK	1197.31	Joback Method
cpg	1560.83	J/molxK	1239.73	Joback Method
cpg	1572.09	J/molxK	1282.15	Joback Method
cpg	1581.64	J/molxK	1324.57	Joback Method
dvisc	0.0001828	Paxs	611.12	Joback Method
dvisc	0.0000907	Paxs	687.61	Joback Method

dvisc	0.0000517	Paxs	764.09	Joback Method
dvisc	0.0000327	Paxs	840.58	Joback Method
dvisc	0.0000223	Paxs	917.07	Joback Method
dvisc	0.0000161	Paxs	993.55	Joback Method
dvisc	0.0000122	Paxs	1070.04	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=U354935&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354935&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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