

# Sebacic acid, 2,3-dimethylphenyl undecyl ester

Inchi:	InChI=1S/C29H48O4/c1-4-5-6-7-8-9-12-15-18-24-32-28(30)22-16-13-10-11-14-17-23-29
InchiKey:	SURDMBAYSQBHLE-UHFFFAOYSA-N
Formula:	C29H48O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	460.69

## Physical Properties

Property code	Value	Unit	Source
gf	-181.39	kJ/mol	Joback Method
hf	-917.90	kJ/mol	Joback Method
hfus	69.70	kJ/mol	Joback Method
hvap	102.06	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.404		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	767.76	kPa	Joback Method
rinpol	3456.00		NIST Webbook
tb	1052.14	K	Joback Method
tc	1297.56	K	Joback Method
tf	612.37	K	Joback Method
vc	1.599	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.39	J/molxK	1052.14	Joback Method
cpg	1450.82	J/molxK	1093.04	Joback Method
cpg	1467.25	J/molxK	1133.95	Joback Method
cpg	1481.77	J/molxK	1174.85	Joback Method
cpg	1494.45	J/molxK	1215.75	Joback Method
cpg	1505.36	J/molxK	1256.65	Joback Method
cpg	1514.58	J/molxK	1297.56	Joback Method
dvisc	0.0001852	Paxs	612.37	Joback Method
dvisc	0.0000969	Paxs	685.66	Joback Method

dvisc	0.0000575	Paxs	758.96	Joback Method
dvisc	0.0000374	Paxs	832.25	Joback Method
dvisc	0.0000261	Paxs	905.55	Joback Method
dvisc	0.0000192	Paxs	978.84	Joback Method
dvisc	0.0000147	Paxs	1052.14	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355214&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355214&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>

## 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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