

# Sebacic acid, 4-methoxyphenyl undecyl ester

**Inchi:** InChI=1S/C28H46O5/c1-3-4-5-6-7-8-11-14-17-24-32-27(29)18-15-12-9-10-13-16-19-28(30)  
**InchiKey:** JLUJDYCDIJZDBF-UHFFFAOYSA-N  
**Formula:** C28H46O5  
**SMILES:** CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(OC)cc1  
**Mol. weight [g/mol]:** 462.66

## Physical Properties

Property code	Value	Unit	Source
gf	-285.18	kJ/mol	Joback Method
hf	-1018.01	kJ/mol	Joback Method
hfus	68.69	kJ/mol	Joback Method
hvap	101.58	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.795		Crippen Method
mvol	402.370	ml/mol	McGowan Method
pc	809.37	kPa	Joback Method
rinpol	3583.00		NIST Webbook
rinpol	3583.00		NIST Webbook
tb	1046.70	K	Joback Method
tc	1290.03	K	Joback Method
tf	610.81	K	Joback Method
vc	1.562	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.39	J/molxK	1046.70	Joback Method
cpg	1415.66	J/molxK	1087.26	Joback Method
cpg	1430.83	J/molxK	1127.81	Joback Method
cpg	1443.96	J/molxK	1168.37	Joback Method
cpg	1455.12	J/molxK	1208.92	Joback Method
cpg	1464.35	J/molxK	1249.48	Joback Method
cpg	1471.71	J/molxK	1290.03	Joback Method
dvisc	0.0001623	Paxs	610.81	Joback Method

dvisc	0.0000840	Paxs	683.46	Joback Method
dvisc	0.0000493	Paxs	756.11	Joback Method
dvisc	0.0000318	Paxs	828.75	Joback Method
dvisc	0.0000220	Paxs	901.40	Joback Method
dvisc	0.0000161	Paxs	974.05	Joback Method
dvisc	0.0000123	Paxs	1046.70	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=U354782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354782&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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