

# Sebacic acid, 4-isopropoxyphenyl undecyl ester

Inchi:	InChI=1S/C30H50O5/c1-4-5-6-7-8-9-12-15-18-25-33-29(31)19-16-13-10-11-14-17-20-30
InchiKey:	OPPXDBCURKPGR-UHFFFAOYSA-N
Formula:	C30H50O5
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]:	490.71

## Physical Properties

Property code	Value	Unit	Source
gf	-270.78	kJ/mol	Joback Method
hf	-1064.57	kJ/mol	Joback Method
hfus	70.35	kJ/mol	Joback Method
hvap	105.65	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.574		Crippen Method
mvol	430.550	ml/mol	McGowan Method
pc	730.86	kPa	Joback Method
rinpol	3545.00		NIST Webbook
tb	1092.02	K	Joback Method
tc	1354.95	K	Joback Method
tf	618.35	K	Joback Method
vc	1.667	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1524.78	J/molxK	1092.02	Joback Method
cpg	1542.27	J/molxK	1135.84	Joback Method
cpg	1557.28	J/molxK	1179.66	Joback Method
cpg	1569.88	J/molxK	1223.48	Joback Method
cpg	1580.15	J/molxK	1267.31	Joback Method
cpg	1588.18	J/molxK	1311.13	Joback Method
cpg	1594.05	J/molxK	1354.95	Joback Method
dvisc	0.0001352	Paxs	618.35	Joback Method
dvisc	0.0000648	Paxs	697.29	Joback Method

dvisc	0.0000361	Paxs	776.24	Joback Method
dvisc	0.0000224	Paxs	855.18	Joback Method
dvisc	0.0000151	Paxs	934.13	Joback Method
dvisc	0.0000108	Paxs	1013.07	Joback Method
dvisc	0.0000081	Paxs	1092.02	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=U354411&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354411&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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