

# Sebacic acid, di(4-isopropoxyphenyl) ester

**Inchi:** InChI=1S/C28H38O6/c1-21(2)31-23-13-17-25(18-14-23)33-27(29)11-9-7-5-6-8-10-12-28  
**InchiKey:** IPDJFIZPGSWTCB-UHFFFAOYSA-N  
**Formula:** C28H38O6  
**SMILES:** CC(C)Oc1ccc(OC(=O)CCCCCCCCC(=O)Oc2ccc(OC(C)C)cc2)cc1  
**Mol. weight [g/mol]:** 470.60

## Physical Properties

Property code	Value	Unit	Source
gf	-292.28	kJ/mol	Joback Method
hf	-935.73	kJ/mol	Joback Method
hfus	56.48	kJ/mol	Joback Method
hvap	106.15	kJ/mol	Joback Method
log10ws	-8.40		Crippen Method
logp	6.893		Crippen Method
mcvol	384.480	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	3457.00		NIST Webbook
tb	1099.90	K	Joback Method
tc	1347.53	K	Joback Method
tf	641.98	K	Joback Method
vc	1.460	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1310.87	J/molxK	1099.90	Joback Method
cpg	1345.40	J/molxK	1306.26	Joback Method
cpg	1342.86	J/molxK	1264.99	Joback Method
cpg	1338.18	J/molxK	1223.71	Joback Method
cpg	1331.31	J/molxK	1182.44	Joback Method
cpg	1322.22	J/molxK	1141.17	Joback Method
cpg	1345.83	J/molxK	1347.53	Joback Method
dvisc	0.0000079	Paxs	1099.90	Joback Method
dvisc	0.0000104	Paxs	1023.58	Joback Method

dvisc	0.0000142	Paxs	947.26	Joback Method
dvisc	0.0000204	Paxs	870.94	Joback Method
dvisc	0.0000316	Paxs	794.62	Joback Method
dvisc	0.0000538	Paxs	718.30	Joback Method
dvisc	0.0001037	Paxs	641.98	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=U354415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354415&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>
<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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