

# Sebacic acid, pentyl phenyl ester

<b>Inchi:</b>	InChI=1S/C21H32O4/c1-2-3-13-18-24-20(22)16-11-6-4-5-7-12-17-21(23)25-19-14-9-8-10
<b>InchiKey:</b>	OHWZOVKDEZDABI-UHFFFAOYSA-N
<b>Formula:</b>	C21H32O4
<b>SMILES:</b>	CCCCCOC(=O)CCCCCCCC(=O)Oc1ccccc1
<b>Mol. weight [g/mol]:</b>	348.48

## Physical Properties

Property code	Value	Unit	Source
gf	-229.49	kJ/mol	Joback Method
hf	-729.84	kJ/mol	Joback Method
hfus	49.76	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.446		Crippen Method
mvol	297.870	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2659.00		NIST Webbook
tb	859.14	K	Joback Method
tc	1059.46	K	Joback Method
tf	497.17	K	Joback Method
vc	1.151	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.74	J/molxK	859.14	Joback Method
cpg	954.16	J/molxK	892.53	Joback Method
cpg	969.42	J/molxK	925.91	Joback Method
cpg	983.54	J/molxK	959.30	Joback Method
cpg	996.55	J/molxK	992.69	Joback Method
cpg	1008.48	J/molxK	1026.07	Joback Method
cpg	1019.36	J/molxK	1059.46	Joback Method
dvisc	0.0006267	Paxs	497.17	Joback Method
dvisc	0.0003221	Paxs	557.50	Joback Method

dvisc	0.0001885	Paxs	617.83	Joback Method
dvisc	0.0001214	Paxs	678.15	Joback Method
dvisc	0.0000840	Paxs	738.48	Joback Method
dvisc	0.0000614	Paxs	798.81	Joback Method
dvisc	0.0000470	Paxs	859.14	Joback Method

## Sources

<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>
<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=U354508&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354508&amp;Units=SI</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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