

# Sebacic acid, 4-methylbenzyl pentyl ester

**Inchi:** InChI=1S/C23H36O4/c1-3-4-11-18-26-22(24)12-9-7-5-6-8-10-13-23(25)27-19-21-16-14-2  
**InchiKey:** FCWJOVCBVWSVHX-UHFFFAOYSA-N  
**Formula:** C23H36O4  
**SMILES:** CCCCCOC(=O)CCCCCCCC(=O)OCc1ccc(C)cc1  
**Mol. weight [g/mol]:** 376.53

## Physical Properties

Property code	Value	Unit	Source
gf	-222.28	kJ/mol	Joback Method
hf	-782.59	kJ/mol	Joback Method
hfus	54.55	kJ/mol	Joback Method
hvap	88.04	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.892		Crippen Method
mvol	326.050	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook
tb	909.88	K	Joback Method
tc	1115.88	K	Joback Method
tf	532.23	K	Joback Method
vc	1.264	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.08	J/molxK	909.88	Joback Method
cpg	1074.86	J/molxK	944.21	Joback Method
cpg	1090.35	J/molxK	978.55	Joback Method
cpg	1104.59	J/molxK	1012.88	Joback Method
cpg	1117.59	J/molxK	1047.21	Joback Method
cpg	1129.40	J/molxK	1081.55	Joback Method
cpg	1140.05	J/molxK	1115.88	Joback Method
dvisc	0.0004311	Paxs	532.23	Joback Method

dvisc	0.0002285	Paxs	595.17	Joback Method
dvisc	0.0001367	Paxs	658.11	Joback Method
dvisc	0.0000895	Paxs	721.06	Joback Method
dvisc	0.0000627	Paxs	784.00	Joback Method
dvisc	0.0000463	Paxs	846.94	Joback Method
dvisc	0.0000357	Paxs	909.88	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=U380705&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380705&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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