

# Sebacic acid, 4-methoxybenzyl propyl ester

**Inchi:** InChI=1S/C21H32O5/c1-3-16-25-20(22)10-8-6-4-5-7-9-11-21(23)26-17-18-12-14-19(24-25)  
**InchiKey:** MXMNYGXWABSSEE-UHFFFAOYSA-N  
**Formula:** C21H32O5  
**SMILES:** CCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC)cc1  
**Mol. weight [g/mol]:** 364.48

## Physical Properties

Property code	Value	Unit	Source
gf	-344.12	kJ/mol	Joback Method
hf	-873.53	kJ/mol	Joback Method
hfus	50.56	kJ/mol	Joback Method
hvap	86.00	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.812		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	886.54	K	Joback Method
tc	1089.96	K	Joback Method
tf	531.92	K	Joback Method
vc	1.169	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.74	J/molxK	886.54	Joback Method
cpg	982.57	J/molxK	920.44	Joback Method
cpg	997.11	J/molxK	954.35	Joback Method
cpg	1010.40	J/molxK	988.25	Joback Method
cpg	1022.43	J/molxK	1022.15	Joback Method
cpg	1033.23	J/molxK	1056.05	Joback Method
cpg	1042.80	J/molxK	1089.96	Joback Method
dvisc	0.0003742	Paxs	531.92	Joback Method

dvisc	0.0002078	Paxs	591.02	Joback Method
dvisc	0.0001284	Paxs	650.13	Joback Method
dvisc	0.0000860	Paxs	709.23	Joback Method
dvisc	0.0000612	Paxs	768.33	Joback Method
dvisc	0.0000458	Paxs	827.44	Joback Method
dvisc	0.0000356	Paxs	886.54	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=U354361&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354361&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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