

# Sebacic acid, 4-phenoxybenzyl propyl ester

**Inchi:** InChI=1S/C26H34O5/c1-2-20-29-25(27)14-10-5-3-4-6-11-15-26(28)30-21-22-16-18-24(1)  
**InchiKey:** NBHFLUCFRQJSST-UHFFFAOYSA-N  
**Formula:** C26H34O5  
**SMILES:** CCCOC(=O)CCCCCCCCC(=O)OCc1ccc(Oc2ccccc2)cc1  
**Mol. weight [g/mol]:** 426.55

## Physical Properties

Property code	Value	Unit	Source
gf	-189.61	kJ/mol	Joback Method
hf	-740.20	kJ/mol	Joback Method
hfus	57.55	kJ/mol	Joback Method
hvap	99.41	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.596		Crippen Method
mvol	350.430	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	3250.00		NIST Webbook
rinpol	3250.00		NIST Webbook
tb	1027.62	K	Joback Method
tc	1258.56	K	Joback Method
tf	614.69	K	Joback Method
vc	1.341	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.89	J/molxK	1027.62	Joback Method
cpg	1178.39	J/molxK	1066.11	Joback Method
cpg	1190.24	J/molxK	1104.60	Joback Method
cpg	1200.46	J/molxK	1143.09	Joback Method
cpg	1209.12	J/molxK	1181.58	Joback Method
cpg	1216.26	J/molxK	1220.07	Joback Method
cpg	1221.93	J/molxK	1258.56	Joback Method
dvisc	0.0001870	Paxs	614.69	Joback Method

dvisc	0.0001032	Paxs	683.51	Joback Method
dvisc	0.0000634	Paxs	752.33	Joback Method
dvisc	0.0000423	Paxs	821.15	Joback Method
dvisc	0.0000301	Paxs	889.98	Joback Method
dvisc	0.0000224	Paxs	958.80	Joback Method
dvisc	0.0000174	Paxs	1027.62	Joback Method

## Sources

<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=U355037&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355037&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>

## Legend

<b>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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