

# Adipic acid, 3-phenoxybenzyl propyl ester

<b>Inchi:</b>	InChI=1S/C22H26O5/c1-2-15-25-21(23)13-6-7-14-22(24)26-17-18-9-8-12-20(16-18)27-1
<b>InchiKey:</b>	LBAXFHWAYMBSTD-UHFFFAOYSA-N
<b>Formula:</b>	C22H26O5
<b>SMILES:</b>	CCCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
<b>Mol. weight [g/mol]:</b>	370.44

## Physical Properties

Property code	Value	Unit	Source
gf	-223.29	kJ/mol	Joback Method
hf	-657.64	kJ/mol	Joback Method
hfus	47.19	kJ/mol	Joback Method
hvap	90.50	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	5.036		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinqol	2778.00		NIST Webbook
tb	936.10	K	Joback Method
tc	1158.31	K	Joback Method
tf	569.61	K	Joback Method
vc	1.117	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.35	J/molxK	936.10	Joback Method
cpg	938.87	J/molxK	973.14	Joback Method
cpg	950.95	J/molxK	1010.17	Joback Method
cpg	961.63	J/molxK	1047.21	Joback Method
cpg	970.94	J/molxK	1084.24	Joback Method
cpg	978.89	J/molxK	1121.28	Joback Method
cpg	985.53	J/molxK	1158.31	Joback Method
dvisc	0.0002967	Paxs	569.61	Joback Method
dvisc	0.0001706	Paxs	630.69	Joback Method

dvisc	0.0001081	Paxs	691.77	Joback Method
dvisc	0.0000738	Paxs	752.86	Joback Method
dvisc	0.0000533	Paxs	813.94	Joback Method
dvisc	0.0000403	Paxs	875.02	Joback Method
dvisc	0.0000316	Paxs	936.10	Joback Method

## Sources

<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=U353811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353811&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>

## 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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