

# Adipic acid, nonyl 3-phenoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C28H38O5/c1-2-3-4-5-6-7-13-21-31-27(29)19-11-12-20-28(30)32-23-24-15-14
<b>InchiKey:</b>	AZYCDCHUNOSEEU-UHFFFAOYSA-N
<b>Formula:</b>	C28H38O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCCC(=O)OCc1cccc(Oc2ccccc2)c1
<b>Mol. weight [g/mol]:</b>	454.60

## Physical Properties

Property code	Value	Unit	Source
gf	-172.77	kJ/mol	Joback Method
hf	-781.48	kJ/mol	Joback Method
hfus	62.73	kJ/mol	Joback Method
hvap	103.86	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.376		Crippen Method
mcvol	378.610	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinsol	3388.00		NIST Webbook
tb	1073.38	K	Joback Method
tc	1314.79	K	Joback Method
tf	637.23	K	Joback Method
vc	1.454	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.96	J/molxK	1073.38	Joback Method
cpg	1300.49	J/molxK	1113.61	Joback Method
cpg	1312.16	J/molxK	1153.85	Joback Method
cpg	1322.05	J/molxK	1194.08	Joback Method
cpg	1330.22	J/molxK	1234.32	Joback Method
cpg	1336.74	J/molxK	1274.55	Joback Method
cpg	1341.67	J/molxK	1314.79	Joback Method
dvisc	0.0001460	Paxs	637.23	Joback Method
dvisc	0.0000790	Paxs	709.92	Joback Method

dvisc	0.0000479	Paxs	782.61	Joback Method
dvisc	0.0000316	Paxs	855.30	Joback Method
dvisc	0.0000223	Paxs	928.00	Joback Method
dvisc	0.0000165	Paxs	1000.69	Joback Method
dvisc	0.0000128	Paxs	1073.38	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=U353819&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353819&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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