

# Glutaric acid, 3-phenoxybenzyl propyl ester

<b>Inchi:</b>	InChI=1S/C21H24O5/c1-2-14-24-20(22)12-7-13-21(23)25-16-17-8-6-11-19(15-17)26-18-
<b>InchiKey:</b>	RHGGOPFULXPWJF-UHFFFAOYSA-N
<b>Formula:</b>	C21H24O5
<b>SMILES:</b>	CCCOC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1
<b>Mol. weight [g/mol]:</b>	356.41

## Physical Properties

Property code	Value	Unit	Source
gf	-231.71	kJ/mol	Joback Method
hf	-637.00	kJ/mol	Joback Method
hfus	44.60	kJ/mol	Joback Method
hvap	88.28	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.646		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook
tb	913.22	K	Joback Method
tc	1135.44	K	Joback Method
tf	558.34	K	Joback Method
vc	1.062	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.73	J/molxK	913.22	Joback Method
cpg	880.24	J/molxK	950.26	Joback Method
cpg	892.35	J/molxK	987.29	Joback Method
cpg	903.09	J/molxK	1024.33	Joback Method
cpg	912.49	J/molxK	1061.37	Joback Method
cpg	920.56	J/molxK	1098.41	Joback Method
cpg	927.34	J/molxK	1135.44	Joback Method
dvisc	0.0003303	Paxs	558.34	Joback Method

dvisc	0.0001920	Paxs	617.49	Joback Method
dvisc	0.0001227	Paxs	676.63	Joback Method
dvisc	0.0000843	Paxs	735.78	Joback Method
dvisc	0.0000612	Paxs	794.93	Joback Method
dvisc	0.0000465	Paxs	854.07	Joback Method
dvisc	0.0000366	Paxs	913.22	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359254&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359254&amp;Units=SI</a>
<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>

## 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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