

# Glutaric acid, 5-methoxy-3-phenylpentyl nonyl ester

Inchi:	InChI=1S/C26H42O5/c1-3-4-5-6-7-8-12-20-30-25(27)16-13-17-26(28)31-22-19-24(18-21
InchiKey:	ZBXPNOQSLZIUBZ-UHFFFAOYSA-N
Formula:	C26H42O5
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCCC(CCOC)c1ccccc1
Mol. weight [g/mol]:	434.61

## Physical Properties

Property code	Value	Unit	Source
gf	-294.83	kJ/mol	Joback Method
hf	-970.54	kJ/mol	Joback Method
hfus	60.38	kJ/mol	Joback Method
hvap	96.08	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	6.204		Crippen Method
mcvol	374.190	ml/mol	McGowan Method
pc	918.27	kPa	Joback Method
rinpol	3124.00		NIST Webbook
tb	995.52	K	Joback Method
tc	1219.91	K	Joback Method
tf	560.75	K	Joback Method
vc	1.444	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1274.13	J/molxK	995.52	Joback Method
cpg	1290.98	J/molxK	1032.92	Joback Method
cpg	1306.09	J/molxK	1070.32	Joback Method
cpg	1319.51	J/molxK	1107.71	Joback Method
cpg	1331.30	J/molxK	1145.11	Joback Method
cpg	1341.49	J/molxK	1182.51	Joback Method
cpg	1350.12	J/molxK	1219.91	Joback Method
dvisc	0.0002634	Paxs	560.75	Joback Method
dvisc	0.0001241	Paxs	633.21	Joback Method

dvisc	0.0000682	Paxs	705.67	Joback Method
dvisc	0.0000419	Paxs	778.13	Joback Method
dvisc	0.0000280	Paxs	850.60	Joback Method
dvisc	0.0000199	Paxs	923.06	Joback Method
dvisc	0.0000149	Paxs	995.52	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=U359535&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359535&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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