

# Glutaric acid, 2-methoxyphenyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C25H40O5/c1-3-4-5-6-7-8-9-10-11-12-15-21-29-24(26)19-16-20-25(27)30-23-
<b>InchiKey:</b>	VNVZFAVKYHDNDG-UHFFFAOYSA-N
<b>Formula:</b>	C25H40O5
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1OC
<b>Mol. weight [g/mol]:</b>	420.58

## Physical Properties

Property code	Value	Unit	Source
gf	-310.44	kJ/mol	Joback Method
hf	-956.09	kJ/mol	Joback Method
hfus	60.92	kJ/mol	Joback Method
hvap	94.90	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.625		Crippen Method
mcvol	360.100	ml/mol	McGowan Method
pc	960.29	kPa	Joback Method
rinpola	3151.00		NIST Webbook
tb	978.06	K	Joback Method
tc	1197.84	K	Joback Method
tf	577.00	K	Joback Method
vc	1.393	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1210.94	J/molxK	978.06	Joback Method
cpg	1227.53	J/molxK	1014.69	Joback Method
cpg	1242.47	J/molxK	1051.32	Joback Method
cpg	1255.79	J/molxK	1087.95	Joback Method
cpg	1267.54	J/molxK	1124.58	Joback Method
cpg	1277.74	J/molxK	1161.21	Joback Method
cpg	1286.41	J/molxK	1197.84	Joback Method
dvisc	0.0002363	Paxs	577.00	Joback Method
dvisc	0.0001258	Paxs	643.84	Joback Method

dvisc	0.0000754	Paxs	710.69	Joback Method
dvisc	0.0000493	Paxs	777.53	Joback Method
dvisc	0.0000345	Paxs	844.37	Joback Method
dvisc	0.0000255	Paxs	911.22	Joback Method
dvisc	0.0000196	Paxs	978.06	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=U358671&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358671&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>mccvol:</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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