

# Glutaric acid, 8-chlorooctyl 5-methyl-2-methoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C21H31ClO5/c1-17-12-13-18(25-2)19(16-17)27-21(24)11-9-10-20(23)26-15-8-
<b>InchiKey:</b>	BGDDDXDFTDOEQB-UHFFFAOYSA-N
<b>Formula:</b>	C21H31ClO5
<b>SMILES:</b>	COc1ccc(C)cc1OC(=O)CCCC(=O)OCCCCCCCCI
<b>Mol. weight [g/mol]:</b>	398.92

## Physical Properties

Property code	Value	Unit	Source
gf	-365.68	kJ/mol	Joback Method
hf	-900.74	kJ/mol	Joback Method
hfus	54.37	kJ/mol	Joback Method
hvap	91.05	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.202		Crippen Method
mvol	315.980	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
tb	928.95	K	Joback Method
tc	1139.76	K	Joback Method
tf	574.36	K	Joback Method
vc	1.218	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.07	J/molxK	928.95	Joback Method
cpg	1051.02	J/molxK	1104.62	Joback Method
cpg	1041.89	J/molxK	1069.49	Joback Method
cpg	1031.44	J/molxK	1034.35	Joback Method
cpg	1019.66	J/molxK	999.22	Joback Method
cpg	1006.54	J/molxK	964.08	Joback Method
cpg	1058.85	J/molxK	1139.76	Joback Method
dvisc	0.0000309	Paxs	928.95	Joback Method

dvisc	0.0000392	Paxs	869.85	Joback Method
dvisc	0.0000514	Paxs	810.75	Joback Method
dvisc	0.0000705	Paxs	751.65	Joback Method
dvisc	0.0001019	Paxs	692.56	Joback Method
dvisc	0.0001579	Paxs	633.46	Joback Method
dvisc	0.0002676	Paxs	574.36	Joback Method

## Sources

<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=U393932&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393932&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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