

# Glutaric acid, 3-chlorophenyl phenethyl ester

<b>Inchi:</b>	InChI=1S/C19H19ClO4/c20-16-8-4-9-17(14-16)24-19(22)11-5-10-18(21)23-13-12-15-6-2
<b>InchiKey:</b>	NLGBBVIIWUUEM-UHFFFAOYSA-N
<b>Formula:</b>	C19H19ClO4
<b>SMILES:</b>	O=C(CCCC(=O)Oc1cccc(Cl)c1)OCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	346.81

## Physical Properties

Property code	Value	Unit	Source
gf	-155.48	kJ/mol	Joback Method
hf	-479.24	kJ/mol	Joback Method
hfus	42.43	kJ/mol	Joback Method
hvap	85.80	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.202		Crippen Method
mcvol	258.170	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	2658.00		NIST Webbook
rinpol	2658.00		NIST Webbook
tb	882.47	K	Joback Method
tc	1111.50	K	Joback Method
tf	543.49	K	Joback Method
vc	0.981	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.62	J/molxK	882.47	Joback Method
cpg	760.32	J/molxK	920.64	Joback Method
cpg	771.77	J/molxK	958.81	Joback Method
cpg	782.02	J/molxK	996.99	Joback Method
cpg	791.10	J/molxK	1035.16	Joback Method
cpg	799.05	J/molxK	1073.33	Joback Method
cpg	805.92	J/molxK	1111.50	Joback Method
dvisc	0.0004741	Paxs	543.49	Joback Method

dvisc	0.0002808	Paxs	599.99	Joback Method
dvisc	0.0001820	Paxs	656.48	Joback Method
dvisc	0.0001264	Paxs	712.98	Joback Method
dvisc	0.0000926	Paxs	769.48	Joback Method
dvisc	0.0000707	Paxs	825.97	Joback Method
dvisc	0.0000560	Paxs	882.47	Joback Method

## Sources

<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=U391794&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391794&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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