

# Glutaric acid, 4-chloro-3-methylphenyl 3-octyl ester

Inchi:	InChI=1S/C20H29ClO4/c1-4-6-7-9-16(5-2)24-19(22)10-8-11-20(23)25-17-12-13-18(21)1
InchiKey:	CAUNHLZGPYTOEW-UHFFFAOYSA-N
Formula:	C20H29ClO4
SMILES:	CCCCC(CC)OC(=O)CCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	368.89

## Physical Properties

Property code	Value	Unit	Source
gf	-271.54	kJ/mol	Joback Method
hf	-753.16	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.626		Crippen Method
mvol	296.020	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	883.21	K	Joback Method
tc	1090.95	K	Joback Method
tf	525.86	K	Joback Method
vc	1.139	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.62	J/molxK	883.21	Joback Method
cpg	919.59	J/molxK	917.83	Joback Method
cpg	933.37	J/molxK	952.46	Joback Method
cpg	945.98	J/molxK	987.08	Joback Method
cpg	957.44	J/molxK	1021.70	Joback Method
cpg	967.77	J/molxK	1056.32	Joback Method
cpg	977.00	J/molxK	1090.95	Joback Method
dvisc	0.0004662	Paxs	525.86	Joback Method

dvisc	0.0002574	Paxs	585.42	Joback Method
dvisc	0.0001586	Paxs	644.98	Joback Method
dvisc	0.0001060	Paxs	704.54	Joback Method
dvisc	0.0000755	Paxs	764.09	Joback Method
dvisc	0.0000565	Paxs	823.65	Joback Method
dvisc	0.0000439	Paxs	883.21	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U391567&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391567&amp;Units=SI</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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