

# Glutaric acid, 3-chlorophenyl 4-chlorobenzyl ester

Inchi:	InChI=1S/C18H16Cl2O4/c19-14-9-7-13(8-10-14)12-23-17(21)5-2-6-18(22)24-16-4-1-3-15
InchiKey:	BJTNVLSYEGLPPL-UHFFFAOYSA-N
Formula:	C18H16Cl2O4
SMILES:	O=C(CCCC(=O)Oc1cccc(Cl)c1)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	367.22

## Physical Properties

Property code	Value	Unit	Source
gf	-185.46	kJ/mol	Joback Method
hf	-485.81	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	88.62	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.812		Crippen Method
mcvol	256.320	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpola	2817.00		NIST Webbook
rinpola	2817.00		NIST Webbook
tb	902.00	K	Joback Method
tc	1137.10	K	Joback Method
tf	574.66	K	Joback Method
vc	0.974	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.95	J/molxK	902.00	Joback Method
cpg	754.54	J/molxK	1097.92	Joback Method
cpg	748.13	J/molxK	1058.74	Joback Method
cpg	740.60	J/molxK	1019.55	Joback Method
cpg	731.92	J/molxK	980.37	Joback Method
cpg	722.05	J/molxK	941.18	Joback Method
cpg	759.86	J/molxK	1137.10	Joback Method
dvisc	0.0000566	Paxs	902.00	Joback Method

dvisc	0.0000703	Paxs	847.44	Joback Method
dvisc	0.0000901	Paxs	792.89	Joback Method
dvisc	0.0001197	Paxs	738.33	Joback Method
dvisc	0.0001664	Paxs	683.77	Joback Method
dvisc	0.0002449	Paxs	629.22	Joback Method
dvisc	0.0003880	Paxs	574.66	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=U391732&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391732&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.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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