

# Glutaric acid, di(3-chlorobenzyl) ester

<b>Inchi:</b>	InChI=1S/C19H18Cl2O4/c20-16-6-1-4-14(10-16)12-24-18(22)8-3-9-19(23)25-13-15-5-2-7
<b>InchiKey:</b>	KQGHVTBGVFLFL-UHFFFAOYSA-N
<b>Formula:</b>	C19H18Cl2O4
<b>SMILES:</b>	O=C(CCCC(=O)OCc1cccc(Cl)c1)OCc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	381.25

## Physical Properties

Property code	Value	Unit	Source
gf	-177.04	kJ/mol	Joback Method
hf	-506.45	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	90.85	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.950		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinqol	3155.00		NIST Webbook
tb	924.88	K	Joback Method
tc	1158.00	K	Joback Method
tf	585.93	K	Joback Method
vc	1.030	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.42	J/molxK	924.88	Joback Method
cpg	778.65	J/molxK	963.73	Joback Method
cpg	788.63	J/molxK	1002.59	Joback Method
cpg	797.41	J/molxK	1041.44	Joback Method
cpg	805.02	J/molxK	1080.29	Joback Method
cpg	811.51	J/molxK	1119.14	Joback Method
cpg	816.89	J/molxK	1158.00	Joback Method
dvisc	0.0003501	Paxs	585.93	Joback Method
dvisc	0.0002184	Paxs	642.42	Joback Method

dvisc	0.0001471	Paxs	698.91	Joback Method
dvisc	0.0001051	Paxs	755.40	Joback Method
dvisc	0.0000787	Paxs	811.90	Joback Method
dvisc	0.0000611	Paxs	868.39	Joback Method
dvisc	0.0000490	Paxs	924.88	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=U377597&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377597&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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