

# Glutaric acid, di(2,2-dichloroethyl) ester

<b>Inchi:</b>	InChI=1S/C9H12Cl4O4/c10-6(11)4-16-8(14)2-1-3-9(15)17-5-7(12)13/h6-7H,1-5H2
<b>InchiKey:</b>	SLUOLGKPMXHICA-UHFFFAOYSA-N
<b>Formula:</b>	C9H12Cl4O4
<b>SMILES:</b>	O=C(CCCC(=O)OCC(Cl)Cl)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	326.00

## Physical Properties

Property code	Value	Unit	Source
gf	-495.54	kJ/mol	Joback Method
hf	-792.21	kJ/mol	Joback Method
hfus	34.38	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.850		Crippen Method
mvol	201.510	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1932.00		NIST Webbook
rinpol	1932.00		NIST Webbook
tb	706.74	K	Joback Method
tc	911.51	K	Joback Method
tf	425.19	K	Joback Method
vc	0.771	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.32	J/molxK	706.74	Joback Method
cpg	478.36	J/molxK	740.87	Joback Method
cpg	487.73	J/molxK	775.00	Joback Method
cpg	496.44	J/molxK	809.12	Joback Method
cpg	504.48	J/molxK	843.25	Joback Method
cpg	511.85	J/molxK	877.38	Joback Method
cpg	518.55	J/molxK	911.51	Joback Method
dvisc	0.0014752	Paxs	425.19	Joback Method

dvisc	0.0007930	Paxs	472.12	Joback Method
dvisc	0.0004769	Paxs	519.04	Joback Method
dvisc	0.0003120	Paxs	565.97	Joback Method
dvisc	0.0002179	Paxs	612.89	Joback Method
dvisc	0.0001601	Paxs	659.82	Joback Method
dvisc	0.0001226	Paxs	706.74	Joback Method

## Sources

<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=U393539&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393539&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>

## 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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<https://www.chemeo.com/cid/124-605-2/Glutaric-acid-di-2-2-dichloroethyl-ester.pdf>

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