

# Glutaric acid, 2,2-dichloroethyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C11H18Cl2O4/c1-8(2)6-16-10(14)4-3-5-11(15)17-7-9(12)13/h8-9H,3-7H2,1-2H
<b>InchiKey:</b>	KULRZZUQLSKUIW-UHFFFAOYSA-N
<b>Formula:</b>	C11H18Cl2O4
<b>SMILES:</b>	CC(C)COC(=O)CCCC(=O)OCC(Cl)Cl
<b>Mol. weight [g/mol]:</b>	285.16

## Physical Properties

Property code	Value	Unit	Source
gf	-454.84	kJ/mol	Joback Method
hf	-802.01	kJ/mol	Joback Method
hfus	31.17	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.703		Crippen Method
mcvol	205.210	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	677.64	K	Joback Method
tc	870.74	K	Joback Method
tf	387.89	K	Joback Method
vc	0.785	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.77	J/molxK	677.64	Joback Method
cpg	534.70	J/molxK	709.82	Joback Method
cpg	546.93	J/molxK	742.01	Joback Method
cpg	558.45	J/molxK	774.19	Joback Method
cpg	569.26	J/molxK	806.37	Joback Method
cpg	579.37	J/molxK	838.56	Joback Method
cpg	588.77	J/molxK	870.74	Joback Method
dvisc	0.0019110	Paxs	387.89	Joback Method

dvisc	0.0009359	Paxs	436.18	Joback Method
dvisc	0.0005285	Paxs	484.47	Joback Method
dvisc	0.0003310	Paxs	532.76	Joback Method
dvisc	0.0002241	Paxs	581.06	Joback Method
dvisc	0.0001610	Paxs	629.35	Joback Method
dvisc	0.0001213	Paxs	677.64	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=U391500&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391500&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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