

# Glutaric acid, 2,2,2-trichloroethyl undecyl ester

Inchi:	InChI=1S/C18H31Cl3O4/c1-2-3-4-5-6-7-8-9-10-14-24-16(22)12-11-13-17(23)25-15-18(19)
InchiKey:	OWLNZTWCALMILZ-UHFFFAOYSA-N
Formula:	C18H31Cl3O4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	417.80

## Physical Properties

Property code	Value	Unit	Source
gf	-400.11	kJ/mol	Joback Method
hf	-960.42	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	85.83	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.144		Crippen Method
mcvol	316.080	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2636.00		NIST Webbook
rinpol	2636.00		NIST Webbook
tb	872.88	K	Joback Method
tc	1072.77	K	Joback Method
tf	529.12	K	Joback Method
vc	1.228	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.85	J/molxK	872.88	Joback Method
cpg	1002.17	J/molxK	1039.45	Joback Method
cpg	991.37	J/molxK	1006.14	Joback Method
cpg	979.68	J/molxK	972.82	Joback Method
cpg	967.05	J/molxK	939.51	Joback Method
cpg	953.46	J/molxK	906.19	Joback Method
cpg	1012.11	J/molxK	1072.77	Joback Method
dvisc	0.0000345	Paxs	872.88	Joback Method

dvisc	0.0000458	Paxs	815.59	Joback Method
dvisc	0.0000633	Paxs	758.29	Joback Method
dvisc	0.0000922	Paxs	701.00	Joback Method
dvisc	0.0001438	Paxs	643.71	Joback Method
dvisc	0.0002444	Paxs	586.41	Joback Method
dvisc	0.0004661	Paxs	529.12	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359352&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359352&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>
<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>

## 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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