

# Glutaric acid, 2,3,5,6-tetrachlorophenyl undecyl ester

<b>Inchi:</b>	InChI=1S/C22H30Cl4O4/c1-2-3-4-5-6-7-8-9-10-14-29-18(27)12-11-13-19(28)30-22-20(29)
<b>InchiKey:</b>	LBLYLIESBDRC-UHFFFAOYSA-N
<b>Formula:</b>	C22H30Cl4O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	500.28

## Physical Properties

Property code	Value	Unit	Source
gf	-307.31	kJ/mol	Joback Method
hf	-859.32	kJ/mol	Joback Method
hfus	67.58	kJ/mol	Joback Method
hvap	105.34	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.450		Crippen Method
mvol	360.920	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	3383.00		NIST Webbook
rinpol	3383.00		NIST Webbook
tb	1051.66	K	Joback Method
tc	1287.64	K	Joback Method
tf	678.20	K	Joback Method
vc	1.403	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.01	J/molxK	1051.66	Joback Method
cpg	1131.32	J/molxK	1248.31	Joback Method
cpg	1125.71	J/molxK	1208.98	Joback Method
cpg	1118.70	J/molxK	1169.65	Joback Method
cpg	1110.27	J/molxK	1130.32	Joback Method
cpg	1100.39	J/molxK	1090.99	Joback Method
cpg	1135.56	J/molxK	1287.64	Joback Method
dvisc	0.0000223	Paxs	1051.66	Joback Method

dvisc	0.0000278	Paxs	989.42	Joback Method
dvisc	0.0000355	Paxs	927.17	Joback Method
dvisc	0.0000471	Paxs	864.93	Joback Method
dvisc	0.0000652	Paxs	802.69	Joback Method
dvisc	0.0000954	Paxs	740.44	Joback Method
dvisc	0.0001497	Paxs	678.20	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=U359326&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359326&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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