

# Glutaric acid, propyl 2,3,4,5-tetrachlorophenyl ester

Inchi:	InChI=1S/C14H14Cl4O4/c1-2-6-21-10(19)4-3-5-11(20)22-9-7-8(15)12(16)14(18)13(9)17
InchiKey:	MKBWVGJUMZBRDCD-UHFFFAOYSA-N
Formula:	C14H14Cl4O4
SMILES:	CCCOC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	388.07

## Physical Properties

Property code	Value	Unit	Source
gf	-374.67	kJ/mol	Joback Method
hf	-694.20	kJ/mol	Joback Method
hfus	46.86	kJ/mol	Joback Method
hvap	87.53	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.329		Crippen Method
mcvol	248.200	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2561.00		NIST Webbook
tb	868.62	K	Joback Method
tc	1090.59	K	Joback Method
tf	588.04	K	Joback Method
vc	0.956	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.71	J/mol×K	868.62	Joback Method
cpg	638.47	J/mol×K	905.61	Joback Method
cpg	647.28	J/mol×K	942.61	Joback Method
cpg	655.12	J/mol×K	979.60	Joback Method
cpg	662.00	J/mol×K	1016.60	Joback Method
cpg	667.90	J/mol×K	1053.59	Joback Method
cpg	672.83	J/mol×K	1090.59	Joback Method
dvisc	0.0003601	Paxs	588.04	Joback Method
dvisc	0.0002511	Paxs	634.80	Joback Method

dvisc	0.0001839	Paxs	681.57	Joback Method
dvisc	0.0001403	Paxs	728.33	Joback Method
dvisc	0.0001105	Paxs	775.09	Joback Method
dvisc	0.0000894	Paxs	821.86	Joback Method
dvisc	0.0000741	Paxs	868.62	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=U360747&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360747&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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