

# Glutaric acid, 2,4,6-trichlorophenyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C19H25Cl3O4/c1-12(10-19(2,3)4)11-25-16(23)6-5-7-17(24)26-18-14(21)8-13(2)
InchiKey:	OGRRWOBLSTRYHGZ-UHFFFAOYSA-N
Formula:	C19H25Cl3O4
SMILES:	CC(COC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)CC(C)(C)C
Mol. weight [g/mol]:	423.76

## Physical Properties

Property code	Value	Unit	Source
gf	-310.61	kJ/mol	Joback Method
hf	-784.22	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	91.93	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.338		Crippen Method
mvol	306.410	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinpol	2657.00		NIST Webbook
rinpol	2657.00		NIST Webbook
tb	936.94	K	Joback Method
tc	1159.57	K	Joback Method
tf	589.37	K	Joback Method
vc	1.169	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.38	J/molxK	936.94	Joback Method
cpg	905.78	J/molxK	974.04	Joback Method
cpg	917.03	J/molxK	1011.15	Joback Method
cpg	927.17	J/molxK	1048.25	Joback Method
cpg	936.24	J/molxK	1085.36	Joback Method
cpg	944.29	J/molxK	1122.46	Joback Method
cpg	951.35	J/molxK	1159.57	Joback Method
dvisc	0.0002619	Paxs	589.37	Joback Method

dvisc	0.0001537	Paxs	647.30	Joback Method
dvisc	0.0000985	Paxs	705.23	Joback Method
dvisc	0.0000675	Paxs	763.15	Joback Method
dvisc	0.0000488	Paxs	821.08	Joback Method
dvisc	0.0000368	Paxs	879.01	Joback Method
dvisc	0.0000288	Paxs	936.94	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=U391541&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391541&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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