

# Glutaric acid, 2-methylpent-3-yl 2,4,5-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C17H21Cl3O4/c1-4-14(10(2)3)23-16(21)6-5-7-17(22)24-15-9-12(19)11(18)8-13
<b>InchiKey:</b>	LBJSTFGARAIAMK-UHFFFAOYSA-N
<b>Formula:</b>	C17H21Cl3O4
<b>SMILES:</b>	CCC(OC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)C(C)C
<b>Mol. weight [g/mol]:</b>	395.70

## Physical Properties

Property code	Value	Unit	Source
gf	-332.73	kJ/mol	Joback Method
hf	-739.47	kJ/mol	Joback Method
hfus	43.78	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.700		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpola	2533.00		NIST Webbook
rinpola	2533.00		NIST Webbook
tb	893.97	K	Joback Method
tc	1113.16	K	Joback Method
tf	549.41	K	Joback Method
vc	1.062	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.04	J/molxK	893.97	Joback Method
cpg	790.01	J/molxK	930.50	Joback Method
cpg	800.84	J/molxK	967.03	Joback Method
cpg	810.55	J/molxK	1003.56	Joback Method
cpg	819.14	J/molxK	1040.10	Joback Method
cpg	826.63	J/molxK	1076.63	Joback Method
cpg	833.02	J/molxK	1113.16	Joback Method
dvisc	0.0004110	Paxs	549.41	Joback Method

dvisc	0.0002402	Paxs	606.84	Joback Method
dvisc	0.0001541	Paxs	664.26	Joback Method
dvisc	0.0001061	Paxs	721.69	Joback Method
dvisc	0.0000772	Paxs	779.12	Joback Method
dvisc	0.0000586	Paxs	836.54	Joback Method
dvisc	0.0000461	Paxs	893.97	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=U392158&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392158&amp;Units=SI</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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