

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

<b>Inchi:</b>	InChI=1S/C16H19Cl3O4/c1-9(2)10(3)22-15(20)5-4-6-16(21)23-14-8-12(18)11(17)7-13(14)
<b>InchiKey:</b>	JWGRINZEDOFRV-UHFFFAOYSA-N
<b>Formula:</b>	C16H19Cl3O4
<b>SMILES:</b>	CC(C)C(C)OC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	381.68

## Physical Properties

Property code	Value	Unit	Source
gf	-341.15	kJ/mol	Joback Method
hf	-718.83	kJ/mol	Joback Method
hfus	41.19	kJ/mol	Joback Method
hvap	86.16	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.310		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook
tb	871.09	K	Joback Method
tc	1091.17	K	Joback Method
tf	538.14	K	Joback Method
vc	1.006	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.52	J/molxK	871.09	Joback Method
cpg	769.49	J/molxK	1054.49	Joback Method
cpg	762.06	J/molxK	1017.81	Joback Method
cpg	753.55	J/molxK	981.13	Joback Method
cpg	743.97	J/molxK	944.45	Joback Method
cpg	733.29	J/molxK	907.77	Joback Method
cpg	775.86	J/molxK	1091.17	Joback Method
dvisc	0.0000534	Paxs	871.09	Joback Method

dvisc	0.0000676	Paxs	815.60	Joback Method
dvisc	0.0000887	Paxs	760.11	Joback Method
dvisc	0.0001213	Paxs	704.62	Joback Method
dvisc	0.0001750	Paxs	649.12	Joback Method
dvisc	0.0002705	Paxs	593.63	Joback Method
dvisc	0.0004572	Paxs	538.14	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=U392157&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392157&amp;Units=SI</a>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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