

# Glutaric acid, 2,4,6-trichlorophenyl hept-4-yl ester

<b>Inchi:</b>	InChI=1S/C18H23Cl3O4/c1-3-6-13(7-4-2)24-16(22)8-5-9-17(23)25-18-14(20)10-12(19)1
<b>InchiKey:</b>	ZJDMMLRUXDCWEZ-UHFFFAOYSA-N
<b>Formula:</b>	C18H23Cl3O4
<b>SMILES:</b>	CCCC(CCC)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	409.73

## Physical Properties

Property code	Value	Unit	Source
gf	-321.87	kJ/mol	Joback Method
hf	-754.83	kJ/mol	Joback Method
hfus	49.89	kJ/mol	Joback Method
hvap	91.00	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.234		Crippen Method
mvol	292.320	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	917.29	K	Joback Method
tc	1134.50	K	Joback Method
tf	575.68	K	Joback Method
vc	1.125	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.79	J/molxK	917.29	Joback Method
cpg	846.87	J/molxK	953.49	Joback Method
cpg	857.80	J/molxK	989.69	Joback Method
cpg	867.60	J/molxK	1025.89	Joback Method
cpg	876.27	J/molxK	1062.09	Joback Method
cpg	883.83	J/molxK	1098.30	Joback Method
cpg	890.30	J/molxK	1134.50	Joback Method
dvisc	0.0003394	Paxs	575.68	Joback Method

dvisc	0.0002067	Paxs	632.62	Joback Method
dvisc	0.0001366	Paxs	689.55	Joback Method
dvisc	0.0000962	Paxs	746.49	Joback Method
dvisc	0.0000711	Paxs	803.42	Joback Method
dvisc	0.0000548	Paxs	860.36	Joback Method
dvisc	0.0000436	Paxs	917.29	Joback Method

## Sources

<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=U392527&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392527&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>h<sub>vap</sub>:</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>m<sub>cvol</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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