

# Glutaric acid, tridec-2-yn-1-yl 2,3,5-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C24H31Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-30-22(28)14-13-15-23(29)31-2
<b>InchiKey:</b>	IUPSJVYNYQRAJK-UHFFFAOYSA-N
<b>Formula:</b>	C24H31Cl3O4
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	489.86

## Physical Properties

Property code	Value	Unit	Source
gf	-66.11	kJ/mol	Joback Method
hf	-601.09	kJ/mol	Joback Method
hfus	72.08	kJ/mol	Joback Method
hvap	106.90	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	7.800		Crippen Method
mvol	368.260	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
rinpol	3378.00		NIST Webbook
rinpol	3378.00		NIST Webbook
tb	1064.01	K	Joback Method
tc	1302.67	K	Joback Method
tf	764.40	K	Joback Method
vc	1.429	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.98	J/molxK	1064.01	Joback Method
cpg	1142.85	J/molxK	1103.79	Joback Method
cpg	1153.21	J/molxK	1143.56	Joback Method
cpg	1162.10	J/molxK	1183.34	Joback Method
cpg	1169.54	J/molxK	1223.12	Joback Method
cpg	1175.59	J/molxK	1262.90	Joback Method
cpg	1180.28	J/molxK	1302.67	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392191&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392191&amp;Units=SI</a>
<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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>rinp:</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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