

# Glutaric acid, 4-chlorophenyl dodecyl ester

**Inchi:** InChI=1S/C23H35ClO4/c1-2-3-4-5-6-7-8-9-10-11-19-27-22(25)13-12-14-23(26)28-21-17-16  
**InchiKey:** UBWARFKKTWANSQ-UHFFFAOYSA-N  
**Formula:** C23H35ClO4  
**SMILES:** CCCCCCCCCCOC(=O)CCCC(=O)Oc1ccc(Cl)cc1  
**Mol. weight [g/mol]:** 410.98

## Physical Properties

Property code	Value	Unit	Source
gf	-234.21	kJ/mol	Joback Method
hf	-798.33	kJ/mol	Joback Method
hfus	58.75	kJ/mol	Joback Method
hvap	92.43	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.880		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpola	3058.00		NIST Webbook
tb	947.31	K	Joback Method
tc	1160.48	K	Joback Method
tf	562.15	K	Joback Method
vc	1.312	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.97	J/molxK	947.31	Joback Method
cpg	1100.59	J/molxK	982.84	Joback Method
cpg	1114.89	J/molxK	1018.37	Joback Method
cpg	1127.90	J/molxK	1053.89	Joback Method
cpg	1139.65	J/molxK	1089.42	Joback Method
cpg	1150.19	J/molxK	1124.95	Joback Method
cpg	1159.55	J/molxK	1160.48	Joback Method
dvisc	0.0003455	Paxs	562.15	Joback Method
dvisc	0.0001870	Paxs	626.34	Joback Method

dvisc	0.0001135	Paxs	690.54	Joback Method
dvisc	0.0000750	Paxs	754.73	Joback Method
dvisc	0.0000529	Paxs	818.92	Joback Method
dvisc	0.0000392	Paxs	883.12	Joback Method
dvisc	0.0000303	Paxs	947.31	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=U359219&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359219&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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