

# Glutaric acid, 3,5-dichlorophenyl ethyl ester

<b>Inchi:</b>	InChI=1S/C13H14Cl2O4/c1-2-18-12(16)4-3-5-13(17)19-11-7-9(14)6-10(15)8-11/h6-8H,2
<b>InchiKey:</b>	YXBWOASZRWBIR-UHFFFAOYSA-N
<b>Formula:</b>	C13H14Cl2O4
<b>SMILES:</b>	CCOC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1
<b>Mol. weight [g/mol]:</b>	305.15

## Physical Properties

Property code	Value	Unit	Source
gf	-339.97	kJ/mol	Joback Method
hf	-619.14	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	75.21	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.632		Crippen Method
mcvol	209.630	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpola	2128.00		NIST Webbook
tb	760.92	K	Joback Method
tc	976.92	K	Joback Method
tf	491.89	K	Joback Method
vc	0.801	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.52	J/molxK	760.92	Joback Method
cpg	585.37	J/molxK	940.92	Joback Method
cpg	577.15	J/molxK	904.92	Joback Method
cpg	568.05	J/molxK	868.92	Joback Method
cpg	558.09	J/molxK	832.92	Joback Method
cpg	547.24	J/molxK	796.92	Joback Method
cpg	592.72	J/molxK	976.92	Joback Method
dvisc	0.0001092	Paxs	760.92	Joback Method
dvisc	0.0001347	Paxs	716.08	Joback Method

dvisc	0.0001708	Paxs	671.24	Joback Method
dvisc	0.0002240	Paxs	626.40	Joback Method
dvisc	0.0003064	Paxs	581.57	Joback Method
dvisc	0.0004416	Paxs	536.73	Joback Method
dvisc	0.0006803	Paxs	491.89	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=U359437&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359437&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>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>mccvol:</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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