

# Glutaric acid, 8-chlorooctyl neopentyl ester

**Inchi:** InChI=1S/C18H33ClO4/c1-18(2,3)15-23-17(21)12-10-11-16(20)22-14-9-7-5-4-6-8-13-19/  
**InchiKey:** ZVBXNQJBENHTCA-UHFFFAOYSA-N  
**Formula:** C18H33ClO4  
**SMILES:** CC(C)(C)COC(=O)CCCC(=O)OCCCCCCCCCI  
**Mol. weight [g/mol]:** 348.90

## Physical Properties

Property code	Value	Unit	Source
gf	-376.25	kJ/mol	Joback Method
hf	-928.94	kJ/mol	Joback Method
hfus	44.73	kJ/mol	Joback Method
hvap	77.06	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.869		Crippen Method
mcvol	291.600	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2358.00		NIST Webbook
rinpol	2358.00		NIST Webbook
tb	798.02	K	Joback Method
tc	986.05	K	Joback Method
tf	469.28	K	Joback Method
vc	1.129	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.37	J/molxK	798.02	Joback Method
cpg	898.95	J/molxK	829.36	Joback Method
cpg	914.54	J/molxK	860.70	Joback Method
cpg	929.19	J/molxK	892.04	Joback Method
cpg	942.91	J/molxK	923.38	Joback Method
cpg	955.73	J/molxK	954.71	Joback Method
cpg	967.69	J/molxK	986.05	Joback Method
dvisc	0.0007842	Paxs	469.28	Joback Method

dvisc	0.0003884	Paxs	524.07	Joback Method
dvisc	0.0002198	Paxs	578.86	Joback Method
dvisc	0.0001372	Paxs	633.65	Joback Method
dvisc	0.0000923	Paxs	688.44	Joback Method
dvisc	0.0000659	Paxs	743.23	Joback Method
dvisc	0.0000492	Paxs	798.02	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=U391620&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391620&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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