

# Glutaric acid, cyclohexylmethyl 2,4,5-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C18H21Cl3O4/c19-13-9-15(21)16(10-14(13)20)25-18(23)8-4-7-17(22)24-11-12
<b>InchiKey:</b>	VTJURLNYXCDFOL-UHFFFAOYSA-N
<b>Formula:</b>	C18H21Cl3O4
<b>SMILES:</b>	O=C(CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)OCC1CCCCC1
<b>Mol. weight [g/mol]:</b>	407.72

## Physical Properties

Property code	Value	Unit	Source
gf	-294.98	kJ/mol	Joback Method
hf	-695.23	kJ/mol	Joback Method
hfus	45.25	kJ/mol	Joback Method
hvap	91.82	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.846		Crippen Method
mcvol	281.460	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2889.00		NIST Webbook
rinpol	2889.00		NIST Webbook
tb	937.28	K	Joback Method
tc	1171.74	K	Joback Method
tf	598.06	K	Joback Method
vc	1.063	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.52	J/molxK	937.28	Joback Method
cpg	838.64	J/molxK	976.36	Joback Method
cpg	849.27	J/molxK	1015.43	Joback Method
cpg	858.44	J/molxK	1054.51	Joback Method
cpg	866.18	J/molxK	1093.58	Joback Method
cpg	872.51	J/molxK	1132.66	Joback Method
cpg	877.44	J/molxK	1171.74	Joback Method
dvisc	0.0003541	Paxs	598.06	Joback Method

dvisc	0.0002212	Paxs	654.60	Joback Method
dvisc	0.0001489	Paxs	711.13	Joback Method
dvisc	0.0001062	Paxs	767.67	Joback Method
dvisc	0.0000794	Paxs	824.21	Joback Method
dvisc	0.0000616	Paxs	880.74	Joback Method
dvisc	0.0000493	Paxs	937.28	Joback Method

## Sources

<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=U392165&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392165&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>

## 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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