

# Glutaric acid, 2,4,6-trichlorophenyl 3-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C18H14Cl3NO6/c19-12-8-14(20)18(15(21)9-12)28-17(24)6-2-5-16(23)27-10-1
<b>InchiKey:</b>	XGDIQGXFASPMQQ-UHFFFAOYSA-N
<b>Formula:</b>	C18H14Cl3NO6
<b>SMILES:</b>	O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	446.67

## Physical Properties

Property code	Value	Unit	Source
gf	-181.10	kJ/mol	Joback Method
hf	-535.25	kJ/mol	Joback Method
hfus	58.43	kJ/mol	Joback Method
hvap	110.92	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	5.374		Crippen Method
mcvol	285.980	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	3364.00		NIST Webbook
rinpol	3364.00		NIST Webbook
tb	1101.23	K	Joback Method
tc	1360.85	K	Joback Method
tf	773.23	K	Joback Method
vc	1.105	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.61	J/molxK	1101.23	Joback Method
cpg	807.76	J/molxK	1144.50	Joback Method
cpg	811.49	J/molxK	1187.77	Joback Method
cpg	813.85	J/molxK	1231.04	Joback Method
cpg	814.87	J/molxK	1274.31	Joback Method
cpg	814.58	J/molxK	1317.58	Joback Method
cpg	813.03	J/molxK	1360.85	Joback Method

# Sources

<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=U393364&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393364&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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