

# Glutaric acid, 2-chloro-6-fluorophenyl trans-4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C21H28ClFO4/c1-21(2,3)14-10-12-15(13-11-14)26-18(24)8-5-9-19(25)27-20-1
InchiKey:	NVGCCTPYSWKYPJ-UHFFFAOYSA-N
Formula:	C21H28ClFO4
SMILES:	CC(C)(C)C1CCC(OC(=O)CCCC(=O)Oc2c(F)cccc2Cl)CC1
Mol. weight [g/mol]:	398.90

## Physical Properties

Property code	Value	Unit	Source
gf	-435.91	kJ/mol	Joback Method
hf	-939.40	kJ/mol	Joback Method
hfus	41.75	kJ/mol	Joback Method
hvap	86.64	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.703		Crippen Method
mvol	301.020	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	917.45	K	Joback Method
tc	1141.28	K	Joback Method
tf	558.28	K	Joback Method
vc	1.139	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.86	J/molxK	917.45	Joback Method
cpg	985.17	J/molxK	954.75	Joback Method
cpg	998.97	J/molxK	992.06	Joback Method
cpg	1011.29	J/molxK	1029.36	Joback Method
cpg	1022.18	J/molxK	1066.67	Joback Method
cpg	1031.69	J/molxK	1103.97	Joback Method
cpg	1039.87	J/molxK	1141.28	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=U393405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393405&amp;Units=SI</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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