

# Glutaric acid, 3-methylbut-2-yl 2,3,4-trifluorophenyl ester

**Inchi:** InChI=1S/C16H19F3O4/c1-9(2)10(3)22-13(20)5-4-6-14(21)23-12-8-7-11(17)15(18)16(12)  
**InchiKey:** INZMIFTUKHTXCH-UHFFFAOYSA-N  
**Formula:** C16H19F3O4  
**SMILES:** CC(C)C(C)OC(=O)CCCC(=O)Oc1ccc(F)c(F)c1F  
**Mol. weight [g/mol]:** 332.31

## Physical Properties

Property code	Value	Unit	Source
gf	-889.79	kJ/mol	Joback Method
hf	-1259.94	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	70.56	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.767		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	756.61	K	Joback Method
tc	947.19	K	Joback Method
tf	450.15	K	Joback Method
vc	0.913	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.03	J/mol×K	756.61	Joback Method
cpg	684.79	J/mol×K	788.37	Joback Method
cpg	697.68	J/mol×K	820.14	Joback Method
cpg	709.70	J/mol×K	851.90	Joback Method
cpg	720.87	J/mol×K	883.66	Joback Method
cpg	731.17	J/mol×K	915.42	Joback Method
cpg	740.63	J/mol×K	947.19	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393635&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393635&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvpap:</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>rinppl:</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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