

# Glutaric acid, 2-fluorophenyl 1,1,1-trifluoroprop-2-yl ester

**Inchi:** InChI=1S/C14H14F4O4/c1-9(14(16,17)18)21-12(19)7-4-8-13(20)22-11-6-3-2-5-10(11)15  
**InchiKey:** ADKVEMNCJJOGEE-UHFFFAOYSA-N  
**Formula:** C14H14F4O4  
**SMILES:** CC(OC(=O)CCCC(=O)Oc1ccccc1F)C(F)(F)F  
**Mol. weight [g/mol]:** 322.25

## Physical Properties

Property code	Value	Unit	Source
gf	-1076.90	kJ/mol	Joback Method
hf	-1395.30	kJ/mol	Joback Method
hfus	32.62	kJ/mol	Joback Method
hvap	63.06	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.395		Crippen Method
mvol	206.320	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
tb	697.37	K	Joback Method
tc	886.33	K	Joback Method
tf	420.58	K	Joback Method
vc	0.815	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.87	J/mol×K	697.37	Joback Method
cpg	587.59	J/mol×K	728.86	Joback Method
cpg	599.49	J/mol×K	760.36	Joback Method
cpg	610.58	J/mol×K	791.85	Joback Method
cpg	620.89	J/mol×K	823.34	Joback Method
cpg	630.45	J/mol×K	854.84	Joback Method
cpg	639.27	J/mol×K	886.33	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=U393655&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393655&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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>rinpola:</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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