

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

<b>Inchi:</b>	InChI=1S/C15H15F3O5/c1-10(15(16,17)18)22-13(20)7-4-8-14(21)23-12-6-3-2-5-11(12)9
<b>InchiKey:</b>	ZOJSRBZDCBRVTP-UHFFFAOYSA-N
<b>Formula:</b>	C15H15F3O5
<b>SMILES:</b>	CC(OC(=O)CCCC(=O)Oc1ccccc1C=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	332.27

## Physical Properties

Property code	Value	Unit	Source
gf	-973.19	kJ/mol	Joback Method
hf	-1305.41	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	72.82	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.069		Crippen Method
mcvol	220.210	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinqol	1941.00		NIST Webbook
tb	769.64	K	Joback Method
tc	967.65	K	Joback Method
tf	473.26	K	Joback Method
vc	0.870	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.20	J/mol×K	769.64	Joback Method
cpg	647.11	J/mol×K	802.64	Joback Method
cpg	658.13	J/mol×K	835.64	Joback Method
cpg	668.29	J/mol×K	868.64	Joback Method
cpg	677.60	J/mol×K	901.64	Joback Method
cpg	686.11	J/mol×K	934.65	Joback Method
cpg	693.83	J/mol×K	967.65	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U390490&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390490&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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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