

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

<b>Inchi:</b>	InChI=1S/C14H10F8O4/c1-5(14(20,21)22)25-6(23)3-2-4-7(24)26-13-11(18)9(16)8(15)10
<b>InchiKey:</b>	IBFZMVVESANPFI-UHFFFAOYSA-N
<b>Formula:</b>	C14H10F8O4
<b>SMILES:</b>	CC(OC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	394.21

## Physical Properties

Property code	Value	Unit	Source
gf	-1894.66	kJ/mol	Joback Method
hf	-2225.62	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	62.44	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	3.952		Crippen Method
mcvol	213.400	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	714.37	K	Joback Method
tc	886.42	K	Joback Method
tf	473.02	K	Joback Method
vc	0.886	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.33	J/molxK	714.37	Joback Method
cpg	613.00	J/molxK	743.04	Joback Method
cpg	623.05	J/molxK	771.72	Joback Method
cpg	632.48	J/molxK	800.39	Joback Method
cpg	641.30	J/molxK	829.07	Joback Method
cpg	649.51	J/molxK	857.74	Joback Method
cpg	657.11	J/molxK	886.42	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U392102&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392102&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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