

# Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,4,5-trichlorophenyl ester

**Inchi:** InChI=1S/C14H12Cl3F3O4/c1-7(14(18,19)20)23-12(21)3-2-4-13(22)24-11-6-9(16)8(15)5  
**InchiKey:** BBPGXQGSJUDJEN-UHFFFAOYSA-N  
**Formula:** C14H12Cl3F3O4  
**SMILES:** CC(OC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)C(F)(F)F  
**Mol. weight [g/mol]:** 407.60

## Physical Properties

Property code	Value	Unit	Source
gf	-937.14	kJ/mol	Joback Method
hf	-1269.35	kJ/mol	Joback Method
hfus	41.36	kJ/mol	Joback Method
hvap	78.35	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.216		Crippen Method
mvol	241.270	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	820.35	K	Joback Method
tc	1029.25	K	Joback Method
tf	534.79	K	Joback Method
vc	0.944	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.96	J/mol×K	820.35	Joback Method
cpg	644.84	J/mol×K	855.17	Joback Method
cpg	653.87	J/mol×K	889.98	Joback Method
cpg	662.06	J/mol×K	924.80	Joback Method
cpg	669.44	J/mol×K	959.62	Joback Method
cpg	676.04	J/mol×K	994.43	Joback Method
cpg	681.87	J/mol×K	1029.25	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=U392153&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392153&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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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