

# Glutaric acid, 2,2-dichloroethyl 2-fluoro-3-trifluoromethylphenyl ester

**Inchi:** InChI=1S/C14H12Cl2F4O4/c15-10(16)7-23-11(21)5-2-6-12(22)24-9-4-1-3-8(13(9)17)14(  
**InchiKey:** FYTYZJLDGHRHNL-UHFFFAOYSA-N  
**Formula:** C14H12Cl2F4O4  
**SMILES:** O=C(CCCC(=O)O)c1cccc(C(F)(F)F)c1F)OCC(Cl)Cl  
**Mol. weight [g/mol]:** 391.14

## Physical Properties

Property code	Value	Unit	Source
gf	-1110.39	kJ/mol	Joback Method
hf	-1438.25	kJ/mol	Joback Method
hfus	40.63	kJ/mol	Joback Method
hvap	72.49	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.267		Crippen Method
mcvol	230.800	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook
tb	777.21	K	Joback Method
tc	975.36	K	Joback Method
tf	492.94	K	Joback Method
vc	0.912	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.52	J/molxK	777.21	Joback Method
cpg	633.12	J/molxK	810.24	Joback Method
cpg	642.90	J/molxK	843.26	Joback Method
cpg	651.88	J/molxK	876.29	Joback Method
cpg	660.09	J/molxK	909.31	Joback Method
cpg	667.55	J/molxK	942.34	Joback Method
cpg	674.29	J/molxK	975.36	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=U393618&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393618&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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