

# Glutaric acid, dec-2-yl 2,3,4-trifluorophenyl ester

Inchi:	InChI=1S/C21H29F3O4/c1-3-4-5-6-7-8-10-15(2)27-18(25)11-9-12-19(26)28-17-14-13-16
InchiKey:	CDNBTQXGWICTQE-UHFFFAOYSA-N
Formula:	C21H29F3O4
SMILES:	CCCCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]:	402.45

## Physical Properties

Property code	Value	Unit	Source
gf	-845.25	kJ/mol	Joback Method
hf	-1357.86	kJ/mol	Joback Method
hfus	54.31	kJ/mol	Joback Method
hvap	82.07	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.862		Crippen Method
mvol	303.180	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	2383.00		NIST Webbook
rinpol	2383.00		NIST Webbook
tb	871.45	K	Joback Method
tc	1068.27	K	Joback Method
tf	521.50	K	Joback Method
vc	1.200	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.17	J/molxK	871.45	Joback Method
cpg	973.52	J/molxK	904.25	Joback Method
cpg	987.74	J/molxK	937.06	Joback Method
cpg	1000.83	J/molxK	969.86	Joback Method
cpg	1012.81	J/molxK	1002.66	Joback Method
cpg	1023.71	J/molxK	1035.47	Joback Method
cpg	1033.53	J/molxK	1068.27	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=U393644&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393644&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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