

# Glutaric acid, 2,2,3,3-tetrafluoropropyl 2-pentyl ester

Inchi:	InChI=1S/C13H20F4O4/c1-3-5-9(2)21-11(19)7-4-6-10(18)20-8-13(16,17)12(14)15/h9,12
InchiKey:	XRVQWJFVTGKHDI-UHFFFAOYSA-N
Formula:	C13H20F4O4
SMILES:	CCCC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	316.29

## Physical Properties

Property code	Value	Unit	Source
gf	-1190.54	kJ/mol	Joback Method
hf	-1605.00	kJ/mol	Joback Method
hfus	32.86	kJ/mol	Joback Method
hvap	57.50	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.332		Crippen Method
mcvol	215.990	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook
tb	642.39	K	Joback Method
tc	807.96	K	Joback Method
tf	355.37	K	Joback Method
vc	0.861	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.03	J/mol×K	642.39	Joback Method
cpg	617.98	J/mol×K	669.98	Joback Method
cpg	631.26	J/mol×K	697.58	Joback Method
cpg	643.86	J/mol×K	725.17	Joback Method
cpg	655.81	J/mol×K	752.77	Joback Method
cpg	667.12	J/mol×K	780.36	Joback Method
cpg	677.80	J/mol×K	807.96	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=U391424&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391424&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>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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