

# Glutaric acid, 2-fluorophenyl hexyl ester

<b>Inchi:</b>	InChI=1S/C17H23FO4/c1-2-3-4-7-13-21-16(19)11-8-12-17(20)22-15-10-6-5-9-14(15)18/
<b>InchiKey:</b>	MAYXEPBFGORDJG-UHFFFAOYSA-N
<b>Formula:</b>	C17H23FO4
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)Oc1ccccc1F
<b>Mol. weight [g/mol]:</b>	310.36

## Physical Properties

Property code	Value	Unit	Source
gf	-467.61	kJ/mol	Joback Method
hf	-854.86	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	73.87	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.025		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpola	2189.00		NIST Webbook
tb	771.87	K	Joback Method
tc	966.58	K	Joback Method
tf	465.20	K	Joback Method
vc	0.946	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.99	J/mol×K	771.87	Joback Method
cpg	726.89	J/mol×K	804.32	Joback Method
cpg	740.82	J/mol×K	836.77	Joback Method
cpg	753.82	J/mol×K	869.23	Joback Method
cpg	765.88	J/mol×K	901.68	Joback Method
cpg	777.03	J/mol×K	934.13	Joback Method
cpg	787.29	J/mol×K	966.58	Joback Method

# Sources

<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=U359032&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359032&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>

# 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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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