

# Glutaric acid, 3-fluorophenyl hexadecyl ester

**Inchi:** InChI=1S/C27H43FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-31-26(29)20-17-21-27(30)  
**InchiKey:** QETVOPGDGILNOT-UHFFFAOYSA-N  
**Formula:** C27H43FO4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1cccc(F)c1  
**Mol. weight [g/mol]:** 450.63

## Physical Properties

Property code	Value	Unit	Source
gf	-383.41	kJ/mol	Joback Method
hf	-1061.26	kJ/mol	Joback Method
hfus	67.99	kJ/mol	Joback Method
hvap	96.13	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.926		Crippen Method
mvol	384.180	ml/mol	McGowan Method
pc	841.62	kPa	Joback Method
rinpol	3239.00		NIST Webbook
rinpol	3239.00		NIST Webbook
tb	1000.67	K	Joback Method
tc	1229.47	K	Joback Method
tf	577.90	K	Joback Method
vc	1.506	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.16	J/molxK	1000.67	Joback Method
cpg	1331.08	J/molxK	1038.80	Joback Method
cpg	1347.32	J/molxK	1076.94	Joback Method
cpg	1361.94	J/molxK	1115.07	Joback Method
cpg	1375.00	J/molxK	1153.21	Joback Method
cpg	1386.57	J/molxK	1191.34	Joback Method
cpg	1396.71	J/molxK	1229.47	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359060&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359060&amp;Units=SI</a>
<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>

# 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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