

# Glutaric acid, 2-(2-fluorophenyl)ethyl pentyl ester

Inchi:	InChI=1S/C18H25FO4/c1-2-3-6-13-22-17(20)10-7-11-18(21)23-14-12-15-8-4-5-9-16(15)
InchiKey:	LMYJQDKZWLGAQA-UHFFFAOYSA-N
Formula:	C18H25FO4
SMILES:	CCCCCOC(=O)CCCC(=O)OCCc1ccccc1F
Mol. weight [g/mol]:	324.39

## Physical Properties

Property code	Value	Unit	Source
gf	-459.19	kJ/mol	Joback Method
hf	-875.50	kJ/mol	Joback Method
hfus	44.68	kJ/mol	Joback Method
hvap	76.09	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.815		Crippen Method
mcvol	257.370	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpola	2283.00		NIST Webbook
tb	794.75	K	Joback Method
tc	989.35	K	Joback Method
tf	476.47	K	Joback Method
vc	1.002	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.80	J/molxK	794.75	Joback Method
cpg	783.99	J/molxK	827.18	Joback Method
cpg	798.18	J/molxK	859.62	Joback Method
cpg	811.39	J/molxK	892.05	Joback Method
cpg	823.64	J/molxK	924.48	Joback Method
cpg	834.94	J/molxK	956.92	Joback Method
cpg	845.31	J/molxK	989.35	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=U377085&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377085&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>

# 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>hvap:</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>rinpola:</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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