

# Glutaric acid, 1-(2-fluorophenyl)ethyl heptyl ester

Inchi:	InChI=1S/C20H29FO4/c1-3-4-5-6-9-15-24-19(22)13-10-14-20(23)25-16(2)17-11-7-8-12-
InchiKey:	VKARRQWIMAQHPI-UHFFFAOYSA-N
Formula:	C20H29FO4
SMILES:	CCCCCCCOC(=O)CCCC(=O)OC(C)c1ccccc1F
Mol. weight [g/mol]:	352.44

## Physical Properties

Property code	Value	Unit	Source
gf	-444.79	kJ/mol	Joback Method
hf	-922.06	kJ/mol	Joback Method
hfus	46.34	kJ/mol	Joback Method
hvap	80.16	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.114		Crippen Method
mcvol	285.550	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpola	2393.00		NIST Webbook
tb	840.07	K	Joback Method
tc	1037.81	K	Joback Method
tf	484.01	K	Joback Method
vc	1.107	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.60	J/molxK	840.07	Joback Method
cpg	901.44	J/molxK	873.03	Joback Method
cpg	916.17	J/molxK	905.98	Joback Method
cpg	929.79	J/molxK	938.94	Joback Method
cpg	942.35	J/molxK	971.90	Joback Method
cpg	953.86	J/molxK	1004.86	Joback Method
cpg	964.34	J/molxK	1037.81	Joback Method

# Sources

<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.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>
<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=U377077&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377077&amp;Units=SI</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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