

# Glutaric acid, 2-fluorophenyl octyl ester

<b>Inchi:</b>	InChI=1S/C19H27FO4/c1-2-3-4-5-6-9-15-23-18(21)13-10-14-19(22)24-17-12-8-7-11-16(
<b>InchiKey:</b>	FTAHQTISAHHVTO-UHFFFAOYSA-N
<b>Formula:</b>	C19H27FO4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1F
<b>Mol. weight [g/mol]:</b>	338.41

## Physical Properties

Property code	Value	Unit	Source
gf	-450.77	kJ/mol	Joback Method
hf	-896.14	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	78.32	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.805		Crippen Method
mvol	271.460	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2422.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	817.63	K	Joback Method
tc	1012.75	K	Joback Method
tf	487.74	K	Joback Method
vc	1.058	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.52	J/mol×K	817.63	Joback Method
cpg	841.99	J/mol×K	850.15	Joback Method
cpg	856.41	J/mol×K	882.67	Joback Method
cpg	869.82	J/mol×K	915.19	Joback Method
cpg	882.22	J/mol×K	947.71	Joback Method
cpg	893.63	J/mol×K	980.23	Joback Method
cpg	904.08	J/mol×K	1012.75	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=U359034&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359034&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>
<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>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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