

# Glutaric acid, decyl 2-fluorophenyl ester

<b>Inchi:</b>	InChI=1S/C21H31FO4/c1-2-3-4-5-6-7-8-11-17-25-20(23)15-12-16-21(24)26-19-14-10-9-
<b>InchiKey:</b>	CLISQQOIGLOPFQ-UHFFFAOYSA-N
<b>Formula:</b>	C21H31FO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)Oc1ccccc1F
<b>Mol. weight [g/mol]:</b>	366.47

## Physical Properties

Property code	Value	Unit	Source
gf	-433.93	kJ/mol	Joback Method
hf	-937.42	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	82.77	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.585		Crippen Method
mcvol	299.640	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinsol	2620.00		NIST Webbook
tb	863.39	K	Joback Method
tc	1061.63	K	Joback Method
tf	510.28	K	Joback Method
vc	1.169	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.43	J/mol×K	863.39	Joback Method
cpg	960.43	J/mol×K	896.43	Joback Method
cpg	975.28	J/mol×K	929.47	Joback Method
cpg	989.02	J/mol×K	962.51	Joback Method
cpg	1001.66	J/mol×K	995.55	Joback Method
cpg	1013.24	J/mol×K	1028.59	Joback Method
cpg	1023.76	J/mol×K	1061.63	Joback Method

# Sources

<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=U359036&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359036&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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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