

# Glutaric acid, 2-fluorophenyl 10-chlorodecyl ester

<b>Inchi:</b>	InChI=1S/C21H30ClFO4/c22-16-9-5-3-1-2-4-6-10-17-26-20(24)14-11-15-21(25)27-19-13
<b>InchiKey:</b>	CTINSQNLZTYWBE-UHFFFAOYSA-N
<b>Formula:</b>	C21H30ClFO4
<b>SMILES:</b>	O=C(CCCC(=O)Oc1ccccc1F)OCCCCCCCCCCI
<b>Mol. weight [g/mol]:</b>	400.91

## Physical Properties

Property code	Value	Unit	Source
gf	-445.86	kJ/mol	Joback Method
hf	-953.16	kJ/mol	Joback Method
hfus	56.65	kJ/mol	Joback Method
hvap	87.16	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.804		Crippen Method
mvol	311.880	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2892.00		NIST Webbook
rinpol	2892.00		NIST Webbook
tb	900.82	K	Joback Method
tc	1105.50	K	Joback Method
tf	540.20	K	Joback Method
vc	1.218	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.49	J/mol×K	900.82	Joback Method
cpg	986.38	J/mol×K	934.93	Joback Method
cpg	1000.10	J/mol×K	969.05	Joback Method
cpg	1012.67	J/mol×K	1003.16	Joback Method
cpg	1024.12	J/mol×K	1037.27	Joback Method
cpg	1034.48	J/mol×K	1071.39	Joback Method
cpg	1043.79	J/mol×K	1105.50	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=U392466&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392466&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>

# 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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