

# Glutaric acid, dodecyl 3-fluorophenyl ester

<b>Inchi:</b>	InChI=1S/C23H35FO4/c1-2-3-4-5-6-7-8-9-10-11-18-27-22(25)16-13-17-23(26)28-21-15-
<b>InchiKey:</b>	NTRSKYRHGZWNKA-UHFFFAOYSA-N
<b>Formula:</b>	C23H35FO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCC(=O)Oc1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	394.52

## Physical Properties

Property code	Value	Unit	Source
gf	-417.09	kJ/mol	Joback Method
hf	-978.70	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	87.22	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.365		Crippen Method
mvol	327.820	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	909.15	K	Joback Method
tc	1113.70	K	Joback Method
tf	532.82	K	Joback Method
vc	1.282	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.16	J/molxK	909.15	Joback Method
cpg	1081.71	J/molxK	943.24	Joback Method
cpg	1096.99	J/molxK	977.33	Joback Method
cpg	1111.03	J/molxK	1011.42	Joback Method
cpg	1123.86	J/molxK	1045.51	Joback Method
cpg	1135.51	J/molxK	1079.61	Joback Method
cpg	1146.01	J/molxK	1113.70	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=U359056&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359056&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>hvp:</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>rinp:</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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