

# Glutaric acid, 2-fluorophenyl 4-chlorobenzyl ester

<b>Inchi:</b>	InChI=1S/C18H16ClFO4/c19-14-10-8-13(9-11-14)12-23-17(21)6-3-7-18(22)24-16-5-2-1-
<b>InchiKey:</b>	VTEQJDKBCIYALM-UHFFFAOYSA-N
<b>Formula:</b>	C18H16ClFO4
<b>SMILES:</b>	O=C(CCCC(=O)Oc1ccccc1F)OCc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	350.77

## Physical Properties

Property code	Value	Unit	Source
gf	-368.34	kJ/mol	Joback Method
hf	-666.18	kJ/mol	Joback Method
hfus	42.53	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.298		Crippen Method
mvol	245.850	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
tb	863.84	K	Joback Method
tc	1088.74	K	Joback Method
tf	545.33	K	Joback Method
vc	0.943	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.25	J/mol×K	863.84	Joback Method
cpg	709.22	J/mol×K	901.32	Joback Method
cpg	720.01	J/mol×K	938.81	Joback Method
cpg	729.68	J/mol×K	976.29	Joback Method
cpg	738.23	J/mol×K	1013.78	Joback Method
cpg	745.71	J/mol×K	1051.26	Joback Method
cpg	752.13	J/mol×K	1088.74	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=U391728&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391728&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.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>

# 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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