

# Glutaric acid, 3-fluorobenzyl propyl ester

<b>Inchi:</b>	InChI=1S/C15H19FO4/c1-2-9-19-14(17)7-4-8-15(18)20-11-12-5-3-6-13(16)10-12/h3,5-6,
<b>InchiKey:</b>	PYPBDYQEGDBIOD-UHFFFAOYSA-N
<b>Formula:</b>	C15H19FO4
<b>SMILES:</b>	CCCOC(=O)CCCC(=O)OCc1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	282.31

## Physical Properties

Property code	Value	Unit	Source
gf	-484.45	kJ/mol	Joback Method
hf	-813.58	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	69.42	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.992		Crippen Method
mcvol	215.100	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinsol	1973.00		NIST Webbook
tb	726.11	K	Joback Method
tc	922.73	K	Joback Method
tf	442.66	K	Joback Method
vc	0.834	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.45	J/mol×K	726.11	Joback Method
cpg	615.65	J/mol×K	758.88	Joback Method
cpg	628.97	J/mol×K	791.65	Joback Method
cpg	641.42	J/mol×K	824.42	Joback Method
cpg	653.01	J/mol×K	857.19	Joback Method
cpg	663.75	J/mol×K	889.96	Joback Method
cpg	673.66	J/mol×K	922.73	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=U376964&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376964&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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