

# Glutaric acid, 3-fluorobenzyl tridecyl ester

**Inchi:** InChI=1S/C25H39FO4/c1-2-3-4-5-6-7-8-9-10-11-12-19-29-24(27)17-14-18-25(28)30-21-2  
**InchiKey:** XQORPCDSMFACAN-UHFFFAOYSA-N  
**Formula:** C25H39FO4  
**SMILES:** CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(F)c1  
**Mol. weight [g/mol]:** 422.57

## Physical Properties

Property code	Value	Unit	Source
gf	-400.25	kJ/mol	Joback Method
hf	-1019.98	kJ/mol	Joback Method
hfus	62.81	kJ/mol	Joback Method
hvap	91.68	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.893		Crippen Method
mvol	356.000	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook
tb	954.91	K	Joback Method
tc	1169.45	K	Joback Method
tf	555.36	K	Joback Method
vc	1.393	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.22	J/molxK	954.91	Joback Method
cpg	1205.40	J/molxK	990.67	Joback Method
cpg	1221.13	J/molxK	1026.42	Joback Method
cpg	1235.46	J/molxK	1062.18	Joback Method
cpg	1248.43	J/molxK	1097.94	Joback Method
cpg	1260.08	J/molxK	1133.69	Joback Method
cpg	1270.46	J/molxK	1169.45	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=U376975&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376975&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>h vap:</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>r in pol:</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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