

# Glutaric acid, 3,4-difluorobenzyl nonyl ester

**Inchi:** InChI=1S/C21H30F2O4/c1-2-3-4-5-6-7-8-14-26-20(24)10-9-11-21(25)27-16-17-12-13-18  
**InchiKey:** NZZBPHJWULUULG-UHFFFAOYSA-N  
**Formula:** C21H30F2O4  
**SMILES:** CCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(F)c(F)c1  
**Mol. weight [g/mol]:** 384.46

## Physical Properties

Property code	Value	Unit	Source
gf	-638.37	kJ/mol	Joback Method
hf	-1145.00	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.472		Crippen Method
mcvol	301.410	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook
tb	867.64	K	Joback Method
tc	1064.57	K	Joback Method
tf	523.39	K	Joback Method
vc	1.188	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.07	J/molxK	867.64	Joback Method
cpg	966.71	J/molxK	900.46	Joback Method
cpg	981.22	J/molxK	933.28	Joback Method
cpg	994.62	J/molxK	966.10	Joback Method
cpg	1006.93	J/molxK	998.92	Joback Method
cpg	1018.17	J/molxK	1031.75	Joback Method
cpg	1028.36	J/molxK	1064.57	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=U377640&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377640&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>
<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>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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