

# Glutaric acid, nonyl pentafluorophenyl ester

<b>Inchi:</b>	InChI=1S/C20H25F5O4/c1-2-3-4-5-6-7-8-12-28-13(26)10-9-11-14(27)29-20-18(24)16(22)
<b>InchiKey:</b>	BLWLPGDUDMOQDF-UHFFFAOYSA-N
<b>Formula:</b>	C20H25F5O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	424.40

## Physical Properties

Property code	Value	Unit	Source
gf	-1260.11	kJ/mol	Joback Method
hf	-1747.10	kJ/mol	Joback Method
hfus	60.63	kJ/mol	Joback Method
hvap	79.93	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	5.752		Crippen Method
mvol	292.630	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	2296.00		NIST Webbook
tb	857.51	K	Joback Method
tc	1049.95	K	Joback Method
tf	551.45	K	Joback Method
vc	1.185	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.62	J/mol×K	857.51	Joback Method
cpg	926.06	J/mol×K	889.58	Joback Method
cpg	939.45	J/mol×K	921.66	Joback Method
cpg	951.81	J/mol×K	953.73	Joback Method
cpg	963.13	J/mol×K	985.80	Joback Method
cpg	973.42	J/mol×K	1017.88	Joback Method
cpg	982.69	J/mol×K	1049.95	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=U359073&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359073&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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