

# Glutaric acid, heptyl pentafluorophenyl ester

<b>Inchi:</b>	InChI=1S/C18H21F5O4/c1-2-3-4-5-6-10-26-11(24)8-7-9-12(25)27-18-16(22)14(20)13(19)
<b>InchiKey:</b>	VDPSIMFBNGLSMU-UHFFFAOYSA-N
<b>Formula:</b>	C18H21F5O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	396.35

## Physical Properties

Property code	Value	Unit	Source
gf	-1276.95	kJ/mol	Joback Method
hf	-1705.82	kJ/mol	Joback Method
hfus	55.45	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	4.971		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpola	2100.00		NIST Webbook
tb	811.75	K	Joback Method
tc	996.55	K	Joback Method
tf	528.91	K	Joback Method
vc	1.073	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.74	J/mol×K	811.75	Joback Method
cpg	809.26	J/mol×K	842.55	Joback Method
cpg	821.89	J/mol×K	873.35	Joback Method
cpg	833.65	J/mol×K	904.15	Joback Method
cpg	844.53	J/mol×K	934.95	Joback Method
cpg	854.53	J/mol×K	965.75	Joback Method
cpg	863.66	J/mol×K	996.55	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=U359071&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359071&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>mccvol:</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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