

# Glutaric acid, hexyl pentafluorophenyl ester

<b>Inchi:</b>	InChI=1S/C17H19F5O4/c1-2-3-4-5-9-25-10(23)7-6-8-11(24)26-17-15(21)13(19)12(18)14
<b>InchiKey:</b>	POQXBNRYQBWLHF-UHFFFAOYSA-N
<b>Formula:</b>	C17H19F5O4
<b>SMILES:</b>	CCCCCOC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	382.32

## Physical Properties

Property code	Value	Unit	Source
gf	-1285.37	kJ/mol	Joback Method
hf	-1685.18	kJ/mol	Joback Method
hfus	52.86	kJ/mol	Joback Method
hvap	73.25	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.581		Crippen Method
mvol	250.360	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rmpol	2009.00		NIST Webbook
tb	788.87	K	Joback Method
tc	971.02	K	Joback Method
tf	517.64	K	Joback Method
vc	1.018	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.11	J/molxK	788.87	Joback Method
cpg	752.16	J/molxK	819.23	Joback Method
cpg	764.39	J/molxK	849.59	Joback Method
cpg	775.81	J/molxK	879.95	Joback Method
cpg	786.43	J/molxK	910.31	Joback Method
cpg	796.23	J/molxK	940.66	Joback Method
cpg	805.22	J/molxK	971.02	Joback Method

# Sources

<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=U359070&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359070&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>

# 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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