

# Glutaric acid, octyl 1-(pentafluorophenyl)ethyl ester

Inchi:	InChI=1S/C21H27F5O4/c1-3-4-5-6-7-8-12-29-14(27)10-9-11-15(28)30-13(2)16-17(22)19
InchiKey:	OPWXRYQJJBYPGF-UHFFFAOYSA-N
Formula:	C21H27F5O4
SMILES:	CCCCCCCCOC(=O)CCCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	438.43

## Physical Properties

Property code	Value	Unit	Source
gf	-1254.13	kJ/mol	Joback Method
hf	-1773.02	kJ/mol	Joback Method
hfus	59.69	kJ/mol	Joback Method
hvap	81.77	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.060		Crippen Method
mvol	306.720	ml/mol	McGowan Method
pc	1038.57	kPa	Joback Method
rinpol	2322.00		NIST Webbook
rinpol	2322.00		NIST Webbook
tb	879.95	K	Joback Method
tc	1077.31	K	Joback Method
tf	547.72	K	Joback Method
vc	1.236	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.21	J/molxK	879.95	Joback Method
cpg	986.08	J/molxK	912.84	Joback Method
cpg	999.80	J/molxK	945.74	Joback Method
cpg	1012.38	J/molxK	978.63	Joback Method
cpg	1023.82	J/molxK	1011.52	Joback Method
cpg	1034.14	J/molxK	1044.42	Joback Method
cpg	1043.33	J/molxK	1077.31	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=U377002&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377002&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>hvp:</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>rinp:</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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