

# Succinic acid, 1-(pentafluorophenyl)ethyl pentyl ester

Inchi:	InChI=1S/C17H19F5O4/c1-3-4-5-8-25-10(23)6-7-11(24)26-9(2)12-13(18)15(20)17(22)16
InchiKey:	UYUXCQUZAUGHME-UHFFFAOYSA-N
Formula:	C17H19F5O4
SMILES:	CCCCCOC(=O)CCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	382.32

## Physical Properties

Property code	Value	Unit	Source
gf	-1287.81	kJ/mol	Joback Method
hf	-1690.46	kJ/mol	Joback Method
hfus	49.33	kJ/mol	Joback Method
hvap	72.86	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.500		Crippen Method
mvol	250.360	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook
tb	788.43	K	Joback Method
tc	971.70	K	Joback Method
tf	502.64	K	Joback Method
vc	1.012	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.67	J/mol×K	788.43	Joback Method
cpg	752.80	J/mol×K	818.98	Joback Method
cpg	765.09	J/mol×K	849.52	Joback Method
cpg	776.56	J/mol×K	880.07	Joback Method
cpg	787.21	J/mol×K	910.61	Joback Method
cpg	797.02	J/mol×K	941.16	Joback Method
cpg	806.00	J/mol×K	971.70	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=U380824&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380824&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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