

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

<b>Inchi:</b>	InChI=1S/C19H23F5O4/c1-3-4-5-6-7-10-27-12(25)8-9-13(26)28-11(2)14-15(20)17(22)19
<b>InchiKey:</b>	MQTRNCPXNMXCMY-UHFFFAOYSA-N
<b>Formula:</b>	C19H23F5O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	410.38

## Physical Properties

Property code	Value	Unit	Source
gf	-1270.97	kJ/mol	Joback Method
hf	-1731.74	kJ/mol	Joback Method
hfus	54.51	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.280		Crippen Method
mvol	278.540	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	2109.00		NIST Webbook
rinpol	2109.00		NIST Webbook
tb	834.19	K	Joback Method
tc	1022.89	K	Joback Method
tf	525.18	K	Joback Method
vc	1.123	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.81	J/mol×K	834.19	Joback Method
cpg	867.81	J/mol×K	865.64	Joback Method
cpg	880.85	J/mol×K	897.09	Joback Method
cpg	892.92	J/mol×K	928.54	Joback Method
cpg	904.02	J/mol×K	959.99	Joback Method
cpg	914.16	J/mol×K	991.44	Joback Method
cpg	923.35	J/mol×K	1022.89	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=U380827&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380827&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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