

# Succinic acid, pentyl 1-phenyl-2,2,2-trifluoroethyl ester

<b>Inchi:</b>	InChI=1S/C17H21F3O4/c1-2-3-7-12-23-14(21)10-11-15(22)24-16(17(18,19)20)13-8-5-4-
<b>InchiKey:</b>	CZXFAJBHRPHTPJ-UHFFFAOYSA-N
<b>Formula:</b>	C17H21F3O4
<b>SMILES:</b>	CCCCCOC(=O)CCC(=O)OC(c1ccccc1)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	346.34

## Physical Properties

Property code	Value	Unit	Source
gf	-847.20	kJ/mol	Joback Method
hf	-1249.64	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	69.89	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.347		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
tb	761.76	K	Joback Method
tc	953.47	K	Joback Method
tf	441.28	K	Joback Method
vc	0.965	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.54	J/molxK	761.76	Joback Method
cpg	744.95	J/molxK	793.71	Joback Method
cpg	758.38	J/molxK	825.66	Joback Method
cpg	770.88	J/molxK	857.62	Joback Method
cpg	782.48	J/molxK	889.57	Joback Method
cpg	793.21	J/molxK	921.52	Joback Method
cpg	803.11	J/molxK	953.47	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=U381571&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381571&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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