

# Succinic acid, 2-fluorophenyl 3-pentyl ester

<b>Inchi:</b>	InChI=1S/C15H19FO4/c1-3-11(4-2)19-14(17)9-10-15(18)20-13-8-6-5-7-12(13)16/h5-8,11
<b>InchiKey:</b>	KENJOWRDVLJPFP-UHFFFAOYSA-N
<b>Formula:</b>	C15H19FO4
<b>SMILES:</b>	CCC(CC)OC(=O)CCC(=O)Oc1ccccc1F
<b>Mol. weight [g/mol]:</b>	282.31

## Physical Properties

Property code	Value	Unit	Source
gf	-486.89	kJ/mol	Joback Method
hf	-818.86	kJ/mol	Joback Method
hfus	33.39	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.243		Crippen Method
mcvol	215.100	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinsol	1830.00		NIST Webbook
tb	725.67	K	Joback Method
tc	925.21	K	Joback Method
tf	427.66	K	Joback Method
vc	0.828	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.99	J/mol×K	725.67	Joback Method
cpg	616.42	J/mol×K	758.93	Joback Method
cpg	629.93	J/mol×K	792.18	Joback Method
cpg	642.53	J/mol×K	825.44	Joback Method
cpg	654.25	J/mol×K	858.69	Joback Method
cpg	665.08	J/mol×K	891.95	Joback Method
cpg	675.03	J/mol×K	925.21	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=U370911&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370911&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>
<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>hvap:</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>rinpola:</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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