

# Succinic acid, 2-fluorophenyl 4-methylpent-2-yl ester

<b>Inchi:</b>	InChI=1S/C16H21FO4/c1-11(2)10-12(3)20-15(18)8-9-16(19)21-14-7-5-4-6-13(14)17/h4-7
<b>InchiKey:</b>	BARJDHRZMNVNIO-UHFFFAOYSA-N
<b>Formula:</b>	C16H21FO4
<b>SMILES:</b>	CC(C)CC(C)OC(=O)CCC(=O)Oc1ccccc1F
<b>Mol. weight [g/mol]:</b>	296.33

## Physical Properties

Property code	Value	Unit	Source
gf	-480.91	kJ/mol	Joback Method
hf	-844.78	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	70.87	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.489		Crippen Method
mvol	229.190	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
tb	748.11	K	Joback Method
tc	948.92	K	Joback Method
tf	423.93	K	Joback Method
vc	0.877	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.27	J/molxK	748.11	Joback Method
cpg	672.26	J/molxK	781.58	Joback Method
cpg	686.26	J/molxK	815.05	Joback Method
cpg	699.29	J/molxK	848.52	Joback Method
cpg	711.36	J/molxK	881.98	Joback Method
cpg	722.47	J/molxK	915.45	Joback Method
cpg	732.65	J/molxK	948.92	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=U390428&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390428&amp;Units=SI</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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