

# Succinic acid, butyl 1-(2-fluorophenyl)ethyl ester

Inchi:	InChI=1S/C16H21FO4/c1-3-4-11-20-15(18)9-10-16(19)21-12(2)13-7-5-6-8-14(13)17/h5-8
InchiKey:	RIAIEKIRBOXGDO-UHFFFAOYSA-N
Formula:	C16H21FO4
SMILES:	CCCCOC(=O)CCC(=O)OC(C)c1ccccc1F
Mol. weight [g/mol]:	296.33

## Physical Properties

Property code	Value	Unit	Source
gf	-478.47	kJ/mol	Joback Method
hf	-839.50	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	71.26	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.553		Crippen Method
mvol	229.190	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
tb	748.55	K	Joback Method
tc	946.59	K	Joback Method
tf	438.93	K	Joback Method
vc	0.883	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.73	J/mol×K	748.55	Joback Method
cpg	671.50	J/mol×K	781.56	Joback Method
cpg	685.32	J/mol×K	814.56	Joback Method
cpg	698.20	J/mol×K	847.57	Joback Method
cpg	710.16	J/mol×K	880.57	Joback Method
cpg	721.20	J/mol×K	913.58	Joback Method
cpg	731.34	J/mol×K	946.59	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=U381392&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381392&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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