

# Succinic acid, 5-fluoro-2-nitrophenyl 3-fluorophenyl ester

**Inchi:** InChI=1S/C16H11F2NO6/c17-10-2-1-3-12(8-10)24-15(20)6-7-16(21)25-14-9-11(18)4-5-1  
**InchiKey:** UFRCZAOGHPCKJS-UHFFFAOYSA-N  
**Formula:** C16H11F2NO6  
**SMILES:** O=C(CCC(=O)Oc1cc(F)ccc1[N+](=O)[O-])Oc1cccc(F)c1  
**Mol. weight [g/mol]:** 351.26

## Physical Properties

Property code	Value	Unit	Source
gf	-542.14	kJ/mol	Joback Method
hf	-827.50	kJ/mol	Joback Method
hfus	47.21	kJ/mol	Joback Method
hvap	91.02	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.164		Crippen Method
mvol	224.620	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	936.74	K	Joback Method
tc	1175.15	K	Joback Method
tf	649.59	K	Joback Method
vc	0.881	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.76	J/molxK	936.74	Joback Method
cpg	669.45	J/molxK	976.48	Joback Method
cpg	676.92	J/molxK	1016.21	Joback Method
cpg	683.19	J/molxK	1055.95	Joback Method
cpg	688.28	J/molxK	1095.68	Joback Method
cpg	692.21	J/molxK	1135.42	Joback Method
cpg	695.01	J/molxK	1175.15	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.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=U357981&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357981&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>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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