

# Succinic acid, 1-(2,6-difluorophenyl)ethyl heptyl ester

Inchi:	InChI=1S/C19H26F2O4/c1-3-4-5-6-7-13-24-17(22)11-12-18(23)25-14(2)19-15(20)9-8-10
InchiKey:	SSGKYFPDODDFKC-UHFFFAOYSA-N
Formula:	C19H26F2O4
SMILES:	CCCCCCCOC(=O)CCC(=O)OC(C)c1c(F)cccc1F
Mol. weight [g/mol]:	356.40

## Physical Properties

Property code	Value	Unit	Source
gf	-657.65	kJ/mol	Joback Method
hf	-1109.00	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.863		Crippen Method
mvol	273.230	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	821.44	K	Joback Method
tc	1015.17	K	Joback Method
tf	485.85	K	Joback Method
vc	1.069	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.81	J/mol×K	821.44	Joback Method
cpg	848.92	J/mol×K	853.73	Joback Method
cpg	863.00	J/mol×K	886.02	Joback Method
cpg	876.06	J/mol×K	918.30	Joback Method
cpg	888.12	J/mol×K	950.59	Joback Method
cpg	899.19	J/mol×K	982.88	Joback Method
cpg	909.29	J/mol×K	1015.17	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=U381423&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381423&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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