

# Succinic acid, 3,4-difluorobenzyl undecyl ester

**Inchi:** InChI=1S/C22H32F2O4/c1-2-3-4-5-6-7-8-9-10-15-27-21(25)13-14-22(26)28-17-18-11-12  
**InchiKey:** NRXYXRBDQXAHRE-UHFFFAOYSA-N  
**Formula:** C22H32F2O4  
**SMILES:** CCCCCCCCCCOC(=O)CCC(=O)OCc1ccc(F)c(F)c1  
**Mol. weight [g/mol]:** 398.48

## Physical Properties

Property code	Value	Unit	Source
gf	-629.95	kJ/mol	Joback Method
hf	-1165.64	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.862		Crippen Method
mvol	315.500	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2627.00		NIST Webbook
rinpol	2627.00		NIST Webbook
tb	890.52	K	Joback Method
tc	1090.98	K	Joback Method
tf	534.66	K	Joback Method
vc	1.244	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.05	J/mol×K	890.52	Joback Method
cpg	1027.01	J/mol×K	923.93	Joback Method
cpg	1041.77	J/mol×K	957.34	Joback Method
cpg	1055.35	J/mol×K	990.75	Joback Method
cpg	1067.77	J/mol×K	1024.16	Joback Method
cpg	1079.07	J/mol×K	1057.57	Joback Method
cpg	1089.26	J/mol×K	1090.98	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=U381749&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381749&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>h vap:</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>r in pol:</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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