

# Succinic acid, 3,4-difluorobenzyl ethyl ester

**Inchi:** InChI=1S/C13H14F2O4/c1-2-18-12(16)5-6-13(17)19-8-9-3-4-10(14)11(15)7-9/h3-4,7H,2,  
**InchiKey:** NEXYAZBZBOQMQR-UHFFFAOYSA-N  
**Formula:** C13H14F2O4  
**SMILES:** CCOC(=O)CCC(=O)OCc1ccc(F)c(F)c1  
**Mol. weight [g/mol]:** 272.24

## Physical Properties

Property code	Value	Unit	Source
gf	-705.73	kJ/mol	Joback Method
hf	-979.88	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.351		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	684.60	K	Joback Method
tc	878.41	K	Joback Method
tf	433.23	K	Joback Method
vc	0.740	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.56	J/molxK	684.60	Joback Method
cpg	515.16	J/molxK	716.90	Joback Method
cpg	527.04	J/molxK	749.20	Joback Method
cpg	538.19	J/molxK	781.50	Joback Method
cpg	548.61	J/molxK	813.81	Joback Method
cpg	558.31	J/molxK	846.11	Joback Method
cpg	567.28	J/molxK	878.41	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=U381739&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381739&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.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>

# 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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