

# Succinic acid, 3,4-difluorobenzyl hexyl ester

<b>Inchi:</b>	InChI=1S/C17H22F2O4/c1-2-3-4-5-10-22-16(20)8-9-17(21)23-12-13-6-7-14(18)15(19)11
<b>InchiKey:</b>	RDTBDPGNDVZDOL-UHFFFAOYSA-N
<b>Formula:</b>	C17H22F2O4
<b>SMILES:</b>	CCCCCCOC(=O)CCC(=O)OCc1ccc(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	328.35

## Physical Properties

Property code	Value	Unit	Source
gf	-672.05	kJ/mol	Joback Method
hf	-1062.44	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	73.71	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.912		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
tb	776.12	K	Joback Method
tc	966.64	K	Joback Method
tf	478.31	K	Joback Method
vc	0.964	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.85	J/molxK	776.12	Joback Method
cpg	733.19	J/molxK	807.87	Joback Method
cpg	746.62	J/molxK	839.63	Joback Method
cpg	759.15	J/molxK	871.38	Joback Method
cpg	770.80	J/molxK	903.13	Joback Method
cpg	781.57	J/molxK	934.89	Joback Method
cpg	791.47	J/molxK	966.64	Joback Method

# Sources

<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=U381745&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381745&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>

# 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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