

# Succinic acid, 2,3,4,5-tetrafluorobenzyl undecyl ester

<b>Inchi:</b>	InChI=1S/C22H30F4O4/c1-2-3-4-5-6-7-8-9-10-13-29-18(27)11-12-19(28)30-15-16-14-17
<b>InchiKey:</b>	DBYLVFNSOMWPFL-UHFFFAOYSA-N
<b>Formula:</b>	C22H30F4O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	434.46

## Physical Properties

Property code	Value	Unit	Source
gf	-1038.83	kJ/mol	Joback Method
hf	-1580.80	kJ/mol	Joback Method
hfus	63.11	kJ/mol	Joback Method
hvap	84.53	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.140		Crippen Method
mcvol	319.040	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinpola	2539.00		NIST Webbook
rinpola	2539.00		NIST Webbook
tb	899.02	K	Joback Method
tc	1100.82	K	Joback Method
tf	560.88	K	Joback Method
vc	1.280	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.05	J/molxK	899.02	Joback Method
cpg	1039.56	J/molxK	932.65	Joback Method
cpg	1053.85	J/molxK	966.29	Joback Method
cpg	1066.93	J/molxK	999.92	Joback Method
cpg	1078.81	J/molxK	1033.55	Joback Method
cpg	1089.52	J/molxK	1067.18	Joback Method
cpg	1099.06	J/molxK	1100.82	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=U381621&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381621&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>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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