

# Succinic acid, decyl 3,4,5-trifluorobenzyl ester

**Inchi:** InChI=1S/C21H29F3O4/c1-2-3-4-5-6-7-8-9-12-27-19(25)10-11-20(26)28-15-16-13-17(22)  
**InchiKey:** ZAYQMGGFAVYVDG-UHFFFAOYSA-N  
**Formula:** C21H29F3O4  
**SMILES:** CCCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1  
**Mol. weight [g/mol]:** 402.45

## Physical Properties

Property code	Value	Unit	Source
gf	-842.81	kJ/mol	Joback Method
hf	-1352.58	kJ/mol	Joback Method
hfus	57.83	kJ/mol	Joback Method
hvap	82.46	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.611		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	871.89	K	Joback Method
tc	1068.26	K	Joback Method
tf	536.50	K	Joback Method
vc	1.206	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.66	J/mol×K	871.89	Joback Method
cpg	973.00	J/mol×K	904.62	Joback Method
cpg	987.21	J/mol×K	937.35	Joback Method
cpg	1000.32	J/mol×K	970.08	Joback Method
cpg	1012.33	J/mol×K	1002.80	Joback Method
cpg	1023.27	J/mol×K	1035.53	Joback Method
cpg	1033.14	J/mol×K	1068.26	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=U382194&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382194&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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