

# Succinic acid, 2,3,6-trifluorobenzyl undecyl ester

Inchi:	InChI=1S/C22H31F3O4/c1-2-3-4-5-6-7-8-9-10-15-28-20(26)13-14-21(27)29-16-17-18(23)
InchiKey:	ARHROUMJZQOXAD-UHFFFAOYSA-N
Formula:	C22H31F3O4
SMILES:	CCCCCCCCCOC(=O)CCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]:	416.47

## Physical Properties

Property code	Value	Unit	Source
gf	-834.39	kJ/mol	Joback Method
hf	-1373.22	kJ/mol	Joback Method
hfus	60.42	kJ/mol	Joback Method
hvap	84.69	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.001		Crippen Method
mcvol	317.270	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	894.77	K	Joback Method
tc	1095.50	K	Joback Method
tf	547.77	K	Joback Method
vc	1.262	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.57	J/molxK	894.77	Joback Method
cpg	1033.28	J/molxK	928.23	Joback Method
cpg	1047.78	J/molxK	961.68	Joback Method
cpg	1061.10	J/molxK	995.14	Joback Method
cpg	1073.24	J/molxK	1028.59	Joback Method
cpg	1084.23	J/molxK	1062.05	Joback Method
cpg	1094.09	J/molxK	1095.50	Joback Method

# Sources

<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>
<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=U381182&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381182&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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