

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

<b>Inchi:</b>	InChI=1S/C20H27F3O4/c1-2-3-4-5-6-7-8-11-26-18(24)9-10-19(25)27-14-15-12-16(21)20
<b>InchiKey:</b>	CBPHWQIWKOZJIK-UHFFFAOYSA-N
<b>Formula:</b>	C20H27F3O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	388.42

## Physical Properties

Property code	Value	Unit	Source
gf	-851.23	kJ/mol	Joback Method
hf	-1331.94	kJ/mol	Joback Method
hfus	55.24	kJ/mol	Joback Method
hvap	80.24	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.221		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	849.01	K	Joback Method
tc	1041.90	K	Joback Method
tf	525.23	K	Joback Method
vc	1.149	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.45	J/molxK	849.01	Joback Method
cpg	913.42	J/molxK	881.16	Joback Method
cpg	927.34	J/molxK	913.31	Joback Method
cpg	940.22	J/molxK	945.45	Joback Method
cpg	952.08	J/molxK	977.60	Joback Method
cpg	962.94	J/molxK	1009.75	Joback Method
cpg	972.79	J/molxK	1041.90	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=U382193&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382193&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>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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