

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

<b>Inchi:</b>	InChI=1S/C14H15F3O4/c1-2-5-20-12(18)3-4-13(19)21-8-9-6-10(15)14(17)11(16)7-9/h6-7
<b>InchiKey:</b>	RCNPGFKQTRFAFZ-UHFFFAOYSA-N
<b>Formula:</b>	C14H15F3O4
<b>SMILES:</b>	CCCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	304.26

## Physical Properties

Property code	Value	Unit	Source
gf	-901.75	kJ/mol	Joback Method
hf	-1208.10	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.880		Crippen Method
mvol	204.550	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1797.00		NIST Webbook
rinpol	1797.00		NIST Webbook
tb	711.73	K	Joback Method
tc	898.61	K	Joback Method
tf	457.61	K	Joback Method
vc	0.814	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.77	J/molxK	711.73	Joback Method
cpg	574.28	J/molxK	742.88	Joback Method
cpg	586.08	J/molxK	774.02	Joback Method
cpg	597.16	J/molxK	805.17	Joback Method
cpg	607.53	J/molxK	836.32	Joback Method
cpg	617.18	J/molxK	867.47	Joback Method
cpg	626.11	J/molxK	898.61	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=U382185&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382185&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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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