

# Succinic acid, 1,1,1-trifluoroprop-2-yl trans-hex-3-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C13H19F3O4/c1-3-4-5-6-9-19-11(17)7-8-12(18)20-10(2)13(14,15)16/h4-5,10H
<b>InchiKey:</b>	KEMQJFHOIBOQSY-SNAWJCMRSA-N
<b>Formula:</b>	C13H19F3O4
<b>SMILES:</b>	CCC=CCCOC(=O)CCC(=O)OC(C)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	296.28

## Physical Properties

Property code	Value	Unit	Source
gf	-913.07	kJ/mol	Joback Method
hf	-1286.39	kJ/mol	Joback Method
hfus	33.50	kJ/mol	Joback Method
hvap	58.67	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.160		Crippen Method
mcvol	209.920	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	1474.00		NIST Webbook
rinpol	1474.00		NIST Webbook
tb	647.72	K	Joback Method
tc	821.37	K	Joback Method
tf	364.70	K	Joback Method
vc	0.829	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.23	J/mol×K	647.72	Joback Method
cpg	587.93	J/mol×K	676.66	Joback Method
cpg	600.92	J/mol×K	705.60	Joback Method
cpg	613.22	J/mol×K	734.55	Joback Method
cpg	624.85	J/mol×K	763.49	Joback Method
cpg	635.83	J/mol×K	792.43	Joback Method
cpg	646.20	J/mol×K	821.37	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=U391107&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391107&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>
<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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