

# Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl but-2-en-1-yl ester

**Inchi:** InChI=1S/C13H14F8O4/c1-2-3-6-24-8(22)4-5-9(23)25-7-11(16,17)13(20,21)12(18,19)10  
**InchiKey:** NXUYBENKVTZHKJ-NSCUHMNNSA-N  
**Formula:** C13H14F8O4  
**SMILES:** CC=CCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)  
**Mol. weight [g/mol]:** 386.24

## Physical Properties

Property code	Value	Unit	Source
gf	-1881.44	kJ/mol	Joback Method
hf	-2284.44	kJ/mol	Joback Method
hfus	34.08	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.600		Crippen Method
mcvol	218.770	ml/mol	McGowan Method
pc	1460.13	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	637.61	K	Joback Method
tc	797.65	K	Joback Method
tf	372.49	K	Joback Method
vc	0.896	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.32	J/mol×K	637.61	Joback Method
cpg	632.54	J/mol×K	664.28	Joback Method
cpg	644.02	J/mol×K	690.96	Joback Method
cpg	654.82	J/mol×K	717.63	Joback Method
cpg	664.95	J/mol×K	744.31	Joback Method
cpg	674.47	J/mol×K	770.98	Joback Method
cpg	683.40	J/mol×K	797.65	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=U391219&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391219&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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