

# Succinic acid, 3-methylbutyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

**Inchi:** InChI=1S/C14H18F8O4/c1-8(2)5-6-25-9(23)3-4-10(24)26-7-12(17,18)14(21,22)13(19,20)

**InchiKey:** AXTWWOICHONWOA-UHFFFAOYSA-N

**Formula:** C14H18F8O4

**SMILES:** CC(C)CCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

**Mol. weight [g/mol]:** 402.28

## Physical Properties

Property code	Value	Unit	Source
gf	-1955.68	kJ/mol	Joback Method
hf	-2427.58	kJ/mol	Joback Method
hfus	32.94	kJ/mol	Joback Method
hvap	53.87	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.070		Crippen Method
mcvol	237.160	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	655.89	K	Joback Method
tc	814.74	K	Joback Method
tf	373.84	K	Joback Method
vc	0.967	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.55	J/mol×K	655.89	Joback Method
cpg	707.97	J/mol×K	682.36	Joback Method
cpg	720.63	J/mol×K	708.84	Joback Method
cpg	732.55	J/mol×K	735.31	Joback Method
cpg	743.78	J/mol×K	761.79	Joback Method
cpg	754.34	J/mol×K	788.26	Joback Method
cpg	764.27	J/mol×K	814.74	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=U370956&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370956&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>

# 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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