

# Sebacic acid, heptadecyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

**Inchi:** InChI=1S/C32H54F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-22-25-43-27(41)23-20-17  
**InchiKey:** BTHBHPDGBJHCGZ-UHFFFAOYSA-N  
**Formula:** C32H54F8O4  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)  
**Mol. weight [g/mol]:** 654.76

## Physical Properties

Property code	Value	Unit	Source
gf	-1801.68	kJ/mol	Joback Method
hf	-2793.82	kJ/mol	Joback Method
hfus	83.09	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-12.20		Crippen Method
logp	11.236		Crippen Method
mvol	490.780	ml/mol	McGowan Method
pc	495.37	kPa	Joback Method
rinpol	3295.00		NIST Webbook
rinpol	3295.00		NIST Webbook
tb	1068.17	K	Joback Method
tc	1406.07	K	Joback Method
tf	591.70	K	Joback Method
vc	1.980	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1787.10	J/molxK	1068.17	Joback Method
cpg	1816.87	J/molxK	1124.49	Joback Method
cpg	1844.00	J/molxK	1180.80	Joback Method
cpg	1869.05	J/molxK	1237.12	Joback Method
cpg	1892.55	J/molxK	1293.44	Joback Method
cpg	1915.03	J/molxK	1349.75	Joback Method
cpg	1937.04	J/molxK	1406.07	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355749&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355749&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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>

# 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>hvpap:</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>rinppl:</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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