

# Octadeca-9,12,15-trienoic acid hexadecyl ester, Z,Z,Z

Inchi:	InChI=1S/C34H62O2/c1-3-5-7-9-11-13-15-17-19-20-22-24-26-28-30-32-34(35)36-33-31-
InchiKey:	SVUULQMAQXFENX-JTBMWNAQSA-N
Formula:	C34H62O2
SMILES:	CCC=CCC=CCC=CCCCCCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	502.85

## Physical Properties

Property code	Value	Unit	Source
gf	242.14	kJ/mol	Joback Method
hf	-638.23	kJ/mol	Joback Method
hfus	87.21	kJ/mol	Joback Method
hvap	100.31	kJ/mol	Joback Method
log10ws	-12.48		Crippen Method
logp	11.600		Crippen Method
mcvol	484.460	ml/mol	McGowan Method
pc	545.90	kPa	Joback Method
rinpol	3522.64		NIST Webbook
rinpol	3522.64		NIST Webbook
tb	1066.09	K	Joback Method
tc	1342.37	K	Joback Method
tf	529.86	K	Joback Method
vc	1.903	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1734.78	J/molxK	1066.09	Joback Method
cpg	1764.23	J/molxK	1112.14	Joback Method
cpg	1792.10	J/molxK	1158.18	Joback Method
cpg	1818.66	J/molxK	1204.23	Joback Method
cpg	1844.18	J/molxK	1250.28	Joback Method
cpg	1868.95	J/molxK	1296.32	Joback Method
cpg	1893.25	J/molxK	1342.37	Joback Method
dvisc	0.0002262	Paxs	529.86	Joback Method

dvisc	0.0000801	Paxs	619.23	Joback Method
dvisc	0.0000369	Paxs	708.60	Joback Method
dvisc	0.0000202	Paxs	797.98	Joback Method
dvisc	0.0000125	Paxs	887.35	Joback Method
dvisc	0.0000084	Paxs	976.72	Joback Method
dvisc	0.0000061	Paxs	1066.09	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=R436727&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R436727&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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