

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

Inchi:	InChI=1S/C36H66O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-
InchiKey:	QQRQYDIHHZSQOG-HLMRNWPHSA-N
Formula:	C36H66O2
SMILES:	CCC=CCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	530.91

## Physical Properties

Property code	Value	Unit	Source
gf	258.98	kJ/mol	Joback Method
hf	-679.51	kJ/mol	Joback Method
hfus	92.39	kJ/mol	Joback Method
hvap	104.76	kJ/mol	Joback Method
log10ws	-13.32		Crippen Method
logp	12.381		Crippen Method
mvol	512.640	ml/mol	McGowan Method
pc	500.03	kPa	Joback Method
rinpol	3723.93		NIST Webbook
rinpol	3723.93		NIST Webbook
tb	1111.85	K	Joback Method
tc	1422.92	K	Joback Method
tf	552.40	K	Joback Method
vc	2.015	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1871.70	J/molxK	1111.85	Joback Method
cpg	1904.80	J/molxK	1163.69	Joback Method
cpg	1936.13	J/molxK	1215.54	Joback Method
cpg	1966.13	J/molxK	1267.38	Joback Method
cpg	1995.21	J/molxK	1319.23	Joback Method
cpg	2023.77	J/molxK	1371.07	Joback Method
cpg	2052.24	J/molxK	1422.92	Joback Method
dvisc	0.0001682	Paxs	552.40	Joback Method

dvisc	0.0000592	Paxs	645.64	Joback Method
dvisc	0.0000271	Paxs	738.88	Joback Method
dvisc	0.0000148	Paxs	832.12	Joback Method
dvisc	0.0000091	Paxs	925.37	Joback Method
dvisc	0.0000061	Paxs	1018.61	Joback Method
dvisc	0.0000044	Paxs	1111.85	Joback Method

## Sources

<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.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>
<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=R436905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R436905&amp;Units=SI</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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