

# Octadeca-9,12-dienoic acid octadecyl ester, Z

<b>Inchi:</b>	InChI=1S/C36H68O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-
<b>InchiKey:</b>	XRHTZVUDPQWCBD-MLWYYCKJSA-N
<b>Formula:</b>	C36H68O2
<b>SMILES:</b>	CCCCC=CCC=CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	532.92

## Physical Properties

Property code	Value	Unit	Source
gf	178.76	kJ/mol	Joback Method
hf	-796.73	kJ/mol	Joback Method
hfus	92.19	kJ/mol	Joback Method
hvap	104.80	kJ/mol	Joback Method
log10ws	-13.46		Crippen Method
logp	12.605		Crippen Method
mvol	516.940	ml/mol	McGowan Method
pc	488.60	kPa	Joback Method
rinpol	3716.27		NIST Webbook
rinpol	3716.27		NIST Webbook
tb	1107.69	K	Joback Method
tc	1426.10	K	Joback Method
tf	557.48	K	Joback Method
vc	2.035	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1899.39	J/molxK	1107.69	Joback Method
cpg	1932.72	J/molxK	1160.76	Joback Method
cpg	1963.73	J/molxK	1213.83	Joback Method
cpg	1992.82	J/molxK	1266.90	Joback Method
cpg	2020.40	J/molxK	1319.96	Joback Method
cpg	2046.86	J/molxK	1373.03	Joback Method
cpg	2072.61	J/molxK	1426.10	Joback Method
dvisc	0.0001798	Paxs	557.48	Joback Method

dvisc	0.0000649	Paxs	649.18	Joback Method
dvisc	0.0000301	Paxs	740.88	Joback Method
dvisc	0.0000166	Paxs	832.59	Joback Method
dvisc	0.0000103	Paxs	924.29	Joback Method
dvisc	0.0000069	Paxs	1015.99	Joback Method
dvisc	0.0000050	Paxs	1107.69	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=R436896&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R436896&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>
<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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