

# Docosanoic acid octadeca-9,12,15-trienyl ester, Z,Z,Z

Inchi:	InChI=1S/C40H74O2/c1-3-5-7-9-11-13-15-17-19-21-22-23-24-26-28-30-32-34-36-38-40
InchiKey:	MUTHJOFVWVWQBLQ-PLYHIOEBSA-N
Formula:	C40H74O2
SMILES:	CCC=CCC=CCG=CCCCCCCCOC(=O)CCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	587.01

## Physical Properties

Property code	Value	Unit	Source
gf	292.66	kJ/mol	Joback Method
hf	-762.07	kJ/mol	Joback Method
hfus	102.75	kJ/mol	Joback Method
hvap	113.66	kJ/mol	Joback Method
log10ws	-14.99		Crippen Method
logp	13.941		Crippen Method
mcvol	569.000	ml/mol	McGowan Method
pc	424.07	kPa	Joback Method
rinpol	4130.13		NIST Webbook
rinpol	4130.13		NIST Webbook
tb	1203.37	K	Joback Method
tc	1610.47	K	Joback Method
tf	597.48	K	Joback Method
vc	2.240	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2150.40	J/molxK	1203.37	Joback Method
cpg	2359.35	J/molxK	1542.62	Joback Method
cpg	2317.22	J/molxK	1474.77	Joback Method
cpg	2276.27	J/molxK	1406.92	Joback Method
cpg	2235.50	J/molxK	1339.07	Joback Method
cpg	2193.88	J/molxK	1271.22	Joback Method
cpg	2403.69	J/molxK	1610.47	Joback Method
dvisc	0.0000023	Paxs	1203.37	Joback Method

dvisc	0.0000032	Paxs	1102.39	Joback Method
dvisc	0.0000048	Paxs	1001.41	Joback Method
dvisc	0.0000078	Paxs	900.42	Joback Method
dvisc	0.0000144	Paxs	799.44	Joback Method
dvisc	0.0000317	Paxs	698.46	Joback Method
dvisc	0.0000913	Paxs	597.48	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=R437260&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R437260&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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