

# Icosa-5,8,11,14-tetraenoic acid hexadec-7-enyl ester

Inchi:	InChI=1S/C36H62O2/c1-3-5-7-9-11-13-15-17-19-20-21-22-24-26-28-30-32-34-36(37)38-
InchiKey:	OSVFMSMUQXQSOI-YHVVKVBXSA-N
Formula:	C36H62O2
SMILES:	CCCCC=CCC=CC=CC=CCCC(=O)OCCCCCCC=CCCCCCCC
Mol. weight [g/mol]:	526.88

## Physical Properties

Property code	Value	Unit	Source
gf	419.42	kJ/mol	Joback Method
hf	-445.07	kJ/mol	Joback Method
hfus	92.79	kJ/mol	Joback Method
hvap	104.68	kJ/mol	Joback Method
log10ws	-13.02		Crippen Method
logp	11.933		Crippen Method
mvol	504.040	ml/mol	McGowan Method
pc	524.12	kPa	Joback Method
rinpol	3642.73		NIST Webbook
tb	1120.17	K	Joback Method
tc	1418.22	K	Joback Method
tf	542.24	K	Joback Method
vc	1.976	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1816.54	J/molxK	1120.17	Joback Method
cpg	1849.43	J/molxK	1169.84	Joback Method
cpg	1881.58	J/molxK	1219.52	Joback Method
cpg	1913.40	J/molxK	1269.19	Joback Method
cpg	1945.35	J/molxK	1318.87	Joback Method
cpg	1977.85	J/molxK	1368.54	Joback Method
cpg	2011.33	J/molxK	1418.22	Joback Method
dvisc	0.0001475	Paxs	542.24	Joback Method
dvisc	0.0000491	Paxs	638.56	Joback Method

dvisc	0.0000218	Paxs	734.88	Joback Method
dvisc	0.0000117	Paxs	831.21	Joback Method
dvisc	0.0000072	Paxs	927.53	Joback Method
dvisc	0.0000048	Paxs	1023.85	Joback Method
dvisc	0.0000034	Paxs	1120.17	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R436841&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R436841&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>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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