

# Icosa-5,8,11,14-tetraenoic acid docosyl ester, Z,Z,Z,Z

Inchi:	InChI=1S/C42H76O2/c1-3-5-7-9-11-13-15-17-19-21-22-23-25-27-29-31-33-35-37-39-41-
InchiKey:	IAYKYXSBKLG MJZ-BHBANYMDSA-N
Formula:	C42H76O2
SMILES:	CCCCC=CCC=CCC=CCC=CCCC(=O)OCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	613.05

## Physical Properties

Property code	Value	Unit	Source
gf	389.72	kJ/mol	Joback Method
hf	-686.13	kJ/mol	Joback Method
hfus	108.13	kJ/mol	Joback Method
hvap	118.07	kJ/mol	Joback Method
log10ws	-15.68		Crippen Method
logp	14.497		Crippen Method
mvol	592.880	ml/mol	McGowan Method
pc	400.64	kPa	Joback Method
rinpol	4270.34		NIST Webbook
tb	1253.29	K	Joback Method
tc	1709.95	K	Joback Method
tf	614.94	K	Joback Method
vc	2.332	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2267.45	J/molxK	1253.29	Joback Method
cpg	2543.17	J/molxK	1633.84	Joback Method
cpg	2481.90	J/molxK	1557.73	Joback Method
cpg	2425.32	J/molxK	1481.62	Joback Method
cpg	2371.80	J/molxK	1405.51	Joback Method
cpg	2319.72	J/molxK	1329.40	Joback Method
cpg	2610.75	J/molxK	1709.95	Joback Method
dvisc	0.0000015	Paxs	1253.29	Joback Method
dvisc	0.0000020	Paxs	1146.90	Joback Method

dvisc	0.0000030	Paxs	1040.51	Joback Method
dvisc	0.0000050	Paxs	934.12	Joback Method
dvisc	0.0000094	Paxs	827.72	Joback Method
dvisc	0.0000210	Paxs	721.33	Joback Method
dvisc	0.0000624	Paxs	614.94	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R437384&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R437384&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>

## 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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