

# docosanyl eicosanoate

**Inchi:** InChI=1S/C42H84O2/c1-3-5-7-9-11-13-15-17-19-21-22-23-25-27-29-31-33-35-37-39-41-43  
**InchiKey:** XRBFFXWJXPXRME-UHFFFAOYSA-N  
**Formula:** C42H84O2  
**SMILES:** CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 621.12

## Physical Properties

Property code	Value	Unit	Source
gf	68.84	kJ/mol	Joback Method
hf	-1155.01	kJ/mol	Joback Method
hfus	107.32	kJ/mol	Joback Method
hvap	118.24	kJ/mol	Joback Method
log10ws	-16.27		Crippen Method
logp	15.393		Crippen Method
mcvol	610.080	ml/mol	McGowan Method
pc	369.25	kPa	Joback Method
rinpol	4346.67		NIST Webbook
rinpol	4346.67		NIST Webbook
tb	1236.65	K	Joback Method
tc	1759.52	K	Joback Method
tf	635.26	K	Joback Method
vc	2.412	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2367.68	J/molxK	1236.65	Joback Method
cpg	2414.29	J/molxK	1323.80	Joback Method
cpg	2454.15	J/molxK	1410.94	Joback Method
cpg	2488.95	J/molxK	1498.09	Joback Method
cpg	2520.37	J/molxK	1585.23	Joback Method
cpg	2550.10	J/molxK	1672.38	Joback Method
cpg	2579.83	J/molxK	1759.52	Joback Method
dvisc	0.0000818	Paxs	635.26	Joback Method

dvisc	0.0000303	Paxs	735.49	Joback Method
dvisc	0.0000142	Paxs	835.72	Joback Method
dvisc	0.0000079	Paxs	935.96	Joback Method
dvisc	0.0000049	Paxs	1036.19	Joback Method
dvisc	0.0000033	Paxs	1136.42	Joback Method
dvisc	0.0000024	Paxs	1236.65	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=R437562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R437562&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>

## Legend

<b>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</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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