

# docosanyl hexadecanoate

<b>Inchi:</b>	InChI=1S/C38H76O2/c1-3-5-7-9-11-13-15-17-18-19-20-21-22-23-25-27-29-31-33-35-37-
<b>InchiKey:</b>	FVFPPJUUBXKFA-UHFFFAOYSA-N
<b>Formula:</b>	C38H76O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	565.01

## Physical Properties

Property code	Value	Unit	Source
gf	35.16	kJ/mol	Joback Method
hf	-1072.45	kJ/mol	Joback Method
hfus	96.96	kJ/mol	Joback Method
hvap	109.34	kJ/mol	Joback Method
log10ws	-14.59		Crippen Method
logp	13.833		Crippen Method
mvol	553.720	ml/mol	McGowan Method
pc	430.43	kPa	Joback Method
rinpol	3947.81		NIST Webbook
rinpol	3947.81		NIST Webbook
tb	1145.13	K	Joback Method
tc	1530.59	K	Joback Method
tf	590.18	K	Joback Method
vc	2.188	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2091.96	J/molxK	1145.13	Joback Method
cpg	2129.57	J/molxK	1209.37	Joback Method
cpg	2162.67	J/molxK	1273.62	Joback Method
cpg	2191.88	J/molxK	1337.86	Joback Method
cpg	2217.78	J/molxK	1402.10	Joback Method
cpg	2240.98	J/molxK	1466.35	Joback Method
cpg	2262.08	J/molxK	1530.59	Joback Method
dvisc	0.0001520	Paxs	590.18	Joback Method

dvisc	0.0000572	Paxs	682.67	Joback Method
dvisc	0.0000272	Paxs	775.16	Joback Method
dvisc	0.0000151	Paxs	867.66	Joback Method
dvisc	0.0000094	Paxs	960.15	Joback Method
dvisc	0.0000064	Paxs	1052.64	Joback Method
dvisc	0.0000046	Paxs	1145.13	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R437577&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R437577&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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