

# Retinyl octanoate

**Inchi:** InChI=1S/C28H44O2/c1-7-8-9-10-11-17-27(29)30-22-20-24(3)15-12-14-23(2)18-19-26-2  
**InchiKey:** AWGMQQGZWRIUJI-UBMBPVGBSA-N  
**Formula:** C28H44O2  
**SMILES:** CCCCCCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C  
**Mol. weight [g/mol]:** 412.65

## Physical Properties

Property code	Value	Unit	Source
gf	284.40	kJ/mol	Joback Method
hf	-312.35	kJ/mol	Joback Method
hfus	55.23	kJ/mol	Joback Method
hvap	87.96	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	8.422		Crippen Method
mvol	380.460	ml/mol	McGowan Method
pc	872.22	kPa	Joback Method
rinpol	3157.00		NIST Webbook
rinpol	3157.00		NIST Webbook
tb	961.64	K	Joback Method
tc	1180.54	K	Joback Method
tf	486.32	K	Joback Method
vc	1.466	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.41	J/molxK	961.64	Joback Method
cpg	1302.27	J/molxK	998.12	Joback Method
cpg	1327.03	J/molxK	1034.61	Joback Method
cpg	1351.89	J/molxK	1071.09	Joback Method
cpg	1377.06	J/molxK	1107.57	Joback Method
cpg	1402.74	J/molxK	1144.05	Joback Method
cpg	1429.15	J/molxK	1180.54	Joback Method

# Sources

<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=R55604&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R55604&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rlnpol:</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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