

# Isopropyl (E)-9-dodecenoate

<b>Inchi:</b>	InChI=1S/C15H28O2/c1-4-5-6-7-8-9-10-11-12-13-15(16)17-14(2)3/h5-6,14H,4,7-13H2,1-
<b>InchiKey:</b>	MMOMOOUGAHBPEF-AATRIKPKSA-N
<b>Formula:</b>	C15H28O2
<b>SMILES:</b>	CCC=CCCCCCCC(=O)OC(C)C
<b>Mol. weight [g/mol]:</b>	240.38

## Physical Properties

Property code	Value	Unit	Source
gf	-80.72	kJ/mol	Joback Method
hf	-485.79	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	57.71	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.635		Crippen Method
mvol	225.350	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
ripol	1884.00		NIST Webbook
ripol	1884.00		NIST Webbook
tb	622.61	K	Joback Method
tc	798.28	K	Joback Method
tf	310.89	K	Joback Method
vc	0.874	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.96	J/molxK	622.61	Joback Method
cpg	618.28	J/molxK	651.89	Joback Method
cpg	634.82	J/molxK	681.17	Joback Method
cpg	650.60	J/molxK	710.44	Joback Method
cpg	665.65	J/molxK	739.72	Joback Method
cpg	679.98	J/molxK	769.00	Joback Method
cpg	693.62	J/molxK	798.28	Joback Method
dvisc	0.0032461	Paxs	310.89	Joback Method

dvisc	0.0012311	Paxs	362.84	Joback Method
dvisc	0.0005952	Paxs	414.80	Joback Method
dvisc	0.0003383	Paxs	466.75	Joback Method
dvisc	0.0002154	Paxs	518.70	Joback Method
dvisc	0.0001488	Paxs	570.66	Joback Method
dvisc	0.0001094	Paxs	622.61	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R488436&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R488436&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>ripol:</b>	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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