

# Tridecanoic acid, 12-methyl-, methyl ester

<b>Other names:</b>	Methyl isomyristate Methyl 12-methyltridecanoate Methyl isotetradecanoate Methyl isotetradecanoate (iso-14:0)
<b>Inchi:</b>	InChI=1S/C15H30O2/c1-14(2)12-10-8-6-4-5-7-9-11-13-15(16)17-3/h14H,4-13H2,1-3H3
<b>InchiKey:</b>	FLESKWMKPOBWDE-UHFFFAOYSA-N
<b>Formula:</b>	C15H30O2
<b>SMILES:</b>	COC(=O)CCCCCCCCCCC(C)C
<b>Mol. weight [g/mol]:</b>	242.40
<b>CAS:</b>	5129-58-8

## Physical Properties

Property code	Value	Unit	Source
gf	-160.94	kJ/mol	Joback Method
hf	-603.01	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.716		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1682.70		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	618.45	K	Joback Method
tc	788.43	K	Joback Method
tf	315.97	K	Joback Method
vc	0.893	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.09	J/molxK	618.45	Joback Method

cpg	702.28	J/molxK	760.10	Joback Method
cpg	687.48	J/molxK	731.77	Joback Method
cpg	671.98	J/molxK	703.44	Joback Method
cpg	655.75	J/molxK	675.11	Joback Method
cpg	638.80	J/molxK	646.78	Joback Method
cpg	716.38	J/molxK	788.43	Joback Method
dvisc	0.0001278	Paxs	618.45	Joback Method
dvisc	0.0001735	Paxs	568.04	Joback Method
dvisc	0.0002499	Paxs	517.62	Joback Method
dvisc	0.0003895	Paxs	467.21	Joback Method
dvisc	0.0006759	Paxs	416.80	Joback Method
dvisc	0.0013649	Paxs	366.38	Joback Method
dvisc	0.0034492	Paxs	315.97	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129588&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129588&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

**vc:** Critical Volume

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