

# 10-Undecynoic acid, methyl ester

<b>Other names:</b>	Methyl 10-undecynoate
<b>Inchi:</b>	InChI=1S/C12H20O2/c1-3-4-5-6-7-8-9-10-11-12(13)14-2/h1H,4-11H2,2H3
<b>InchiKey:</b>	TXFNJLOAXFOJGK-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O2
<b>SMILES:</b>	C#CCCCCCCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	196.29
<b>CAS:</b>	2777-66-4

## Physical Properties

Property code	Value	Unit	Source
gf	39.31	kJ/mol	Joback Method
hf	-243.91	kJ/mol	Joback Method
hfus	32.60	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.913		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1446.30		NIST Webbook
rinpol	1446.30		NIST Webbook
tb	540.37	K	Joback Method
tc	720.11	K	Joback Method
tf	344.13	K	Joback Method
vc	0.694	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.67	J/molxK	540.37	Joback Method
cpg	440.30	J/molxK	570.33	Joback Method
cpg	454.31	J/molxK	600.28	Joback Method
cpg	467.70	J/molxK	630.24	Joback Method
cpg	480.50	J/molxK	660.20	Joback Method
cpg	492.72	J/molxK	690.16	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=C2777664&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2777664&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.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>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>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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