

# Undec-10-ynoic acid, tetradecyl ester

<b>Inchi:</b>	InChI=1S/C25H46O2/c1-3-5-7-9-11-13-14-15-16-18-20-22-24-27-25(26)23-21-19-17-12-
<b>InchiKey:</b>	AGXFKXFGJDTHNJ-UHFFFAOYSA-N
<b>Formula:</b>	C25H46O2
<b>SMILES:</b>	C#CCCCCCCCC(=O)OCCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	378.63

## Physical Properties

Property code	Value	Unit	Source
gf	148.77	kJ/mol	Joback Method
hf	-512.23	kJ/mol	Joback Method
hfus	66.27	kJ/mol	Joback Method
hvap	80.26	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.985		Crippen Method
mvol	361.950	ml/mol	McGowan Method
pc	852.97	kPa	Joback Method
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
tb	837.81	K	Joback Method
tc	1025.90	K	Joback Method
tf	490.64	K	Joback Method
vc	1.421	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.34	J/mol×K	837.81	Joback Method
cpg	1183.27	J/mol×K	869.16	Joback Method
cpg	1203.07	J/mol×K	900.51	Joback Method
cpg	1221.78	J/mol×K	931.85	Joback Method
cpg	1239.46	J/mol×K	963.20	Joback Method
cpg	1256.14	J/mol×K	994.55	Joback Method
cpg	1271.87	J/mol×K	1025.90	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406167&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406167&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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