

# 9-Decenoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi:	InChI=1S/C14H25NO/c1-4-5-6-7-8-9-10-11-13-15-14(2,3)12-16-13/h4H,1,5-12H2,2-3H3
InchiKey:	WCWKMKCASOICGI-UHFFFAOYSA-N
Formula:	C14H25NO
SMILES:	C=CCCCCCCCC1=NC(C)(C)CO1
Mol. weight [g/mol]:	223.35

## Physical Properties

Property code	Value	Unit	Source
gf	236.89	kJ/mol	Joback Method
hf	-145.86	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	56.87	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.110		Crippen Method
mcvol	204.510	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpola	1512.30		NIST Webbook
rinpola	1512.30		NIST Webbook
tb	616.71	K	Joback Method
tc	818.13	K	Joback Method
tf	391.97	K	Joback Method
vc	0.795	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.47	J/mol×K	616.71	Joback Method
cpg	583.68	J/mol×K	650.28	Joback Method
cpg	601.90	J/mol×K	683.85	Joback Method
cpg	619.25	J/mol×K	717.42	Joback Method
cpg	635.82	J/mol×K	750.99	Joback Method
cpg	651.69	J/mol×K	784.56	Joback Method
cpg	666.97	J/mol×K	818.13	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=U333578&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333578&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>hvpap:</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>rinppl:</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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