

# trans-13-Octadecenoic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi:	InChI=1S/C22H41NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-23-22(2,3)20-2
InchiKey:	LAPZQVVNBSJZOY-BQYQJAHWSA-N
Formula:	C22H41NO
SMILES:	CCCC=CCCCCCCCCCCCC1=NC(C)(C)CO1
Mol. weight [g/mol]:	335.57

## Physical Properties

Property code	Value	Unit	Source
gf	296.63	kJ/mol	Joback Method
hf	-319.19	kJ/mol	Joback Method
hfus	54.52	kJ/mol	Joback Method
hvap	75.30	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.231		Crippen Method
mvol	317.230	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2314.80		NIST Webbook
tb	807.23	K	Joback Method
tc	1001.28	K	Joback Method
tf	478.81	K	Joback Method
vc	1.242	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.00	J/mol×K	807.23	Joback Method
cpg	1054.08	J/mol×K	839.57	Joback Method
cpg	1075.38	J/mol×K	871.91	Joback Method
cpg	1096.01	J/mol×K	904.26	Joback Method
cpg	1116.07	J/mol×K	936.60	Joback Method
cpg	1135.68	J/mol×K	968.94	Joback Method
cpg	1154.95	J/mol×K	1001.28	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333614&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333614&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>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>rinpola:</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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