

# cis-8,11,14-Eicosatrienoic acid, 4,4-dimethyloxazoline (dmox) derivative

**Inchi:** InChI=1S/C24H41NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-25-24(2,3,4)/1H,2H,3H,4H,5H,6H,7H,8H,9H,10H,11H,12H,13H,14H,15H,16H,17H,18H,19H,20H,21H,23H,25H,26H,27H,28H,29H,30H,31H,32H,33H,34H,35H,36H,37H,38H,39H,40H,41H,42H,43H,44H,45H,46H,47H,48H,49H,50H,51H,52H,53H,54H,55H,56H,57H,58H,59H,60H,61H,62H,63H,64H,65H,66H,67H,68H,69H,70H,71H,72H,73H,74H,75H,76H,77H,78H,79H,80H,81H,82H,83H,84H,85H,86H,87H,88H,89H,90H,91H,92H,93H,94H,95H,96H,97H,98H,99H,100H

**InchiKey:** KWSGHOHBFKRYBP-ORZIMQNZSA-N

**Formula:** C24H41NO

**SMILES:** CCCCCC=CCC=CCG=CCCCCCCC1=NC(C)(C)CO1

**Mol. weight [g/mol]:** 359.59

## Physical Properties

Property code	Value	Unit	Source
gf	473.91	kJ/mol	Joback Method
hf	-126.03	kJ/mol	Joback Method
hfus	60.11	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.563		Crippen Method
mcvol	336.810	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	2487.80		NIST Webbook
rinpol	2487.80		NIST Webbook
tb	861.31	K	Joback Method
tc	1064.86	K	Joback Method
tf	491.19	K	Joback Method
vc	1.315	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.13	J/molxK	861.31	Joback Method
cpg	1129.61	J/molxK	895.23	Joback Method
cpg	1151.54	J/molxK	929.16	Joback Method
cpg	1173.06	J/molxK	963.08	Joback Method
cpg	1194.34	J/molxK	997.01	Joback Method
cpg	1215.53	J/molxK	1030.93	Joback Method
cpg	1236.79	J/molxK	1064.86	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333610&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333610&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>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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