

# (E,Z)-2,13-octadecadienal

Inchi:	InChI=1S/C18H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h5-6,16-18H,2-4
InchiKey:	NCFULMZVHNTQOK-RAPDCGKPSA-N
Formula:	C18H32O
SMILES:	CCCC=CCCCCCCCCCC=CC=O
Mol. weight [g/mol]:	264.45

## Physical Properties

Property code	Value	Unit	Source
gf	161.60	kJ/mol	Joback Method
hf	-265.99	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.999		Crippen Method
mcvol	257.450	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2064.00		NIST Webbook
ripol	2481.00		NIST Webbook
tb	668.22	K	Joback Method
tc	841.93	K	Joback Method
tf	324.46	K	Joback Method
vc	1.020	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.37	J/molxK	668.22	Joback Method
cpg	732.27	J/molxK	697.17	Joback Method
cpg	749.33	J/molxK	726.12	Joback Method
cpg	765.60	J/molxK	755.08	Joback Method
cpg	781.12	J/molxK	784.03	Joback Method
cpg	795.94	J/molxK	812.98	Joback Method
cpg	810.09	J/molxK	841.93	Joback Method

dvisc	0.0030745	Paxs	324.46	Joback Method
dvisc	0.0011371	Paxs	381.75	Joback Method
dvisc	0.0005452	Paxs	439.05	Joback Method
dvisc	0.0003097	Paxs	496.34	Joback Method
dvisc	0.0001978	Paxs	553.63	Joback Method
dvisc	0.0001374	Paxs	610.93	Joback Method
dvisc	0.0001016	Paxs	668.22	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=R399163&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R399163&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>dvisc:</b>	Dynamic viscosity
<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>mvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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