

# 2-Ethyleicosanoic acid

<b>Inchi:</b>	InChI=1S/C22H44O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(4-2)22(23)24
<b>InchiKey:</b>	MBFSRSJRTRVYJN-UHFFFAOYSA-N
<b>Formula:</b>	C22H44O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCC(C)C(=O)O
<b>Mol. weight [g/mol]:</b>	340.58

## Physical Properties

Property code	Value	Unit	Source
gf	-133.82	kJ/mol	Joback Method
hf	-767.50	kJ/mol	Joback Method
hfus	54.90	kJ/mol	Joback Method
hvap	87.60	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.749		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	997.02	kPa	Joback Method
rinpol	2377.00		NIST Webbook
rinpol	2377.00		NIST Webbook
tb	848.37	K	Joback Method
tc	1038.91	K	Joback Method
tf	433.45	K	Joback Method
vc	1.286	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.51	J/molxK	848.37	Joback Method
cpg	1098.03	J/molxK	880.13	Joback Method
cpg	1116.49	J/molxK	911.88	Joback Method
cpg	1133.93	J/molxK	943.64	Joback Method
cpg	1150.42	J/molxK	975.39	Joback Method
cpg	1165.99	J/molxK	1007.15	Joback Method
cpg	1180.69	J/molxK	1038.91	Joback Method
dvisc	0.0015132	Paxs	433.45	Joback Method

dvisc	0.0003761	Paxs	502.60	Joback Method
dvisc	0.0001309	Paxs	571.76	Joback Method
dvisc	0.0000572	Paxs	640.91	Joback Method
dvisc	0.0000294	Paxs	710.06	Joback Method
dvisc	0.0000170	Paxs	779.22	Joback Method
dvisc	0.0000107	Paxs	848.37	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R435591&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R435591&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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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