

# 5-Eicosenoic acid, methyl ester

<b>Inchi:</b>	InChI=1S/C22H42O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(23)24-2
<b>InchiKey:</b>	AEFLJPWAIVIDGO-ISLYRVAYSAN
<b>Formula:</b>	C22H42O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCC=CCCC(=O)OC
<b>Mol. weight [g/mol]:</b>	338.57

## Physical Properties

Property code	Value	Unit	Source
gf	-19.34	kJ/mol	Joback Method
hf	-624.99	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.367		Crippen Method
mvol	323.980	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook
tb	783.21	K	Joback Method
tc	962.10	K	Joback Method
tf	404.78	K	Joback Method
vc	1.272	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.83	J/molxK	783.21	Joback Method
cpg	1026.84	J/molxK	813.03	Joback Method
cpg	1045.86	J/molxK	842.84	Joback Method
cpg	1063.93	J/molxK	872.66	Joback Method
cpg	1081.08	J/molxK	902.47	Joback Method
cpg	1097.36	J/molxK	932.29	Joback Method
cpg	1112.80	J/molxK	962.10	Joback Method
dvisc	0.0012526	Paxs	404.78	Joback Method

dvisc	0.0005052	Paxs	467.85	Joback Method
dvisc	0.0002528	Paxs	530.92	Joback Method
dvisc	0.0001465	Paxs	593.99	Joback Method
dvisc	0.0000943	Paxs	657.07	Joback Method
dvisc	0.0000656	Paxs	720.14	Joback Method
dvisc	0.0000483	Paxs	783.21	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R99389&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R99389&amp;Units=SI</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>mcvol:</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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