

# 1-Methyl-2-methoxyethyl heptadecanoate

<b>Inchi:</b>	InChI=1S/C21H42O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(22)24-20(2)19-23-3
<b>InchiKey:</b>	ZNCFZCYDGRDWOI-UHFFFAOYSA-N
<b>Formula:</b>	C21H42O3
<b>SMILES:</b>	CCCCCCCCCCCCCCCC(=O)OC(C)COC
<b>Mol. weight [g/mol]:</b>	342.56

## Physical Properties

Property code	Value	Unit	Source
gf	-215.42	kJ/mol	Joback Method
hf	-859.07	kJ/mol	Joback Method
hfus	50.60	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.436		Crippen Method
mcvol	320.060	ml/mol	McGowan Method
pc	978.40	kPa	Joback Method
rinsol	2293.00		NIST Webbook
rinsol	2293.00		NIST Webbook
tb	778.15	K	Joback Method
tc	955.58	K	Joback Method
tf	405.82	K	Joback Method
vc	1.248	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.15	J/molxK	778.15	Joback Method
cpg	1023.21	J/molxK	807.72	Joback Method
cpg	1042.25	J/molxK	837.29	Joback Method
cpg	1060.26	J/molxK	866.86	Joback Method
cpg	1077.28	J/molxK	896.43	Joback Method
cpg	1093.32	J/molxK	926.00	Joback Method
cpg	1108.40	J/molxK	955.58	Joback Method
dvisc	0.0012278	Paxs	405.82	Joback Method

dvisc	0.0004891	Paxs	467.88	Joback Method
dvisc	0.0002417	Paxs	529.93	Joback Method
dvisc	0.0001385	Paxs	591.99	Joback Method
dvisc	0.0000882	Paxs	654.04	Joback Method
dvisc	0.0000607	Paxs	716.10	Joback Method
dvisc	0.0000444	Paxs	778.15	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=R540133&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R540133&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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