

# 4-Pentenoic acid, 2-methyl-, octadecyl ester

**Inchi:** InChI=1S/C24H46O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-26-24(25)23(3)  
**InchiKey:** NKWULGVORMGRDS-UHFFFAOYSA-N  
**Formula:** C24H46O2  
**SMILES:** C=CCC(C)C(=O)OCCCCCCCCCCCCCCCCCCC  
**Mol. weight [g/mol]:** 366.62

## Physical Properties

Property code	Value	Unit	Source
gf	2.68	kJ/mol	Joback Method
hf	-663.34	kJ/mol	Joback Method
hfus	55.90	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	8.003		Crippen Method
mvol	352.160	ml/mol	McGowan Method
pc	851.97	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	821.05	K	Joback Method
tc	1005.63	K	Joback Method
tf	415.64	K	Joback Method
vc	1.379	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.59	J/mol×K	821.05	Joback Method
cpg	1150.67	J/mol×K	851.81	Joback Method
cpg	1170.61	J/mol×K	882.58	Joback Method
cpg	1189.46	J/mol×K	913.34	Joback Method
cpg	1207.27	J/mol×K	944.10	Joback Method
cpg	1224.06	J/mol×K	974.86	Joback Method
cpg	1239.88	J/mol×K	1005.63	Joback Method
dvisc	0.0013025	Paxs	415.64	Joback Method

dvisc	0.0004891	Paxs	483.21	Joback Method
dvisc	0.0002336	Paxs	550.78	Joback Method
dvisc	0.0001311	Paxs	618.35	Joback Method
dvisc	0.0000824	Paxs	685.91	Joback Method
dvisc	0.0000563	Paxs	753.48	Joback Method
dvisc	0.0000410	Paxs	821.05	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=U406121&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406121&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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