

# Octadecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester

Other names:	Glycerol, 2-octadecanoate, diacetate
Inchi:	InChI=1S/C25H46O6/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-25(28)31-24(20-29
InchiKey:	FLZMENQJJSKDLW-UHFFFAOYSA-N
Formula:	C25H46O6
SMILES:	CCCCCCCCCCCCCCCCC(=O)OC(COC(C)=O)COC(C)=O
Mol. weight [g/mol]:	442.63
CAS:	55401-62-2

## Physical Properties

Property code	Value	Unit	Source
gf	-544.58	kJ/mol	Joback Method
hf	-1299.01	kJ/mol	Joback Method
hfus	65.34	kJ/mol	Joback Method
hvap	98.32	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.286		Crippen Method
mcvol	385.430	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
tb	999.83	K	Joback Method
tc	1233.94	K	Joback Method
tf	572.99	K	Joback Method
vc	1.502	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.11	J/molxK	999.83	Joback Method
cpg	1350.36	J/molxK	1038.85	Joback Method
cpg	1366.61	J/molxK	1077.87	Joback Method
cpg	1380.90	J/molxK	1116.88	Joback Method
cpg	1393.25	J/molxK	1155.90	Joback Method
cpg	1403.71	J/molxK	1194.92	Joback Method
cpg	1412.30	J/molxK	1233.94	Joback Method
dvisc	0.0002679	Paxs	572.99	Joback Method

dvisc	0.0001286	Paxs	644.13	Joback Method
dvisc	0.0000714	Paxs	715.27	Joback Method
dvisc	0.0000441	Paxs	786.41	Joback Method
dvisc	0.0000295	Paxs	857.55	Joback Method
dvisc	0.0000210	Paxs	928.69	Joback Method
dvisc	0.0000157	Paxs	999.83	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55401622&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55401622&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>cp<sub>g</sub>:</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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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