

# Hexanoic acid, octadecyl ester

<b>Other names:</b>	Octadecyl caproate
<b>Inchi:</b>	InChI=1S/C24H48O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-21-23-26-24(25)22-2
<b>InchiKey:</b>	GQKMJPMHAWIENG-UHFFFAOYSA-N
<b>Formula:</b>	C24H48O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)CCCCC
<b>Mol. weight [g/mol]:</b>	368.64
<b>CAS:</b>	41927-67-7

## Physical Properties

Property code	Value	Unit	Source
gf	-82.72	kJ/mol	Joback Method
hf	-783.49	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	8.371		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2569.00		NIST Webbook
tb	824.81	K	Joback Method
tc	1009.81	K	Joback Method
tf	432.40	K	Joback Method
vc	1.403	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.81	J/molxK	824.81	Joback Method
cpg	1253.86	J/molxK	978.97	Joback Method
cpg	1236.63	J/molxK	948.14	Joback Method
cpg	1218.34	J/molxK	917.31	Joback Method
cpg	1198.97	J/molxK	886.48	Joback Method
cpg	1178.47	J/molxK	855.64	Joback Method
cpg	1270.08	J/molxK	1009.81	Joback Method

dvisc	0.0000418	Paxs	824.81	Joback Method
dvisc	0.0000568	Paxs	759.41	Joback Method
dvisc	0.0000818	Paxs	694.01	Joback Method
dvisc	0.0001271	Paxs	628.61	Joback Method
dvisc	0.0002188	Paxs	563.20	Joback Method
dvisc	0.0004342	Paxs	497.80	Joback Method
dvisc	0.0010603	Paxs	432.40	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=C41927677&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41927677&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>mvol:</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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