

# Decanoic acid, octyl ester

<b>Other names:</b>	octyl decanoate
<b>Inchi:</b>	InChI=1S/C18H36O2/c1-3-5-7-9-11-12-14-16-18(19)20-17-15-13-10-8-6-4-2/h3-17H2,1-2
<b>InchiKey:</b>	HRPZGPXWSVHWPB-UHFFFAOYSA-N
<b>Formula:</b>	C18H36O2
<b>SMILES:</b>	CCCCCCCCC(=O)OCCCCCCCC
<b>Mol. weight [g/mol]:</b>	284.48
<b>CAS:</b>	2306-92-5

## Physical Properties

Property code	Value	Unit	Source
gf	-133.24	kJ/mol	Joback Method
hf	-659.65	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	64.82	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	6.031		Crippen Method
mvol	271.920	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	1979.60		NIST Webbook
tb	687.53	K	Joback Method
tc	855.83	K	Joback Method
tf	272.45 ± 3.00	K	NIST Webbook
vc	1.067	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.92	J/mol×K	687.53	Joback Method
cpg	875.72	J/mol×K	827.78	Joback Method
cpg	860.14	J/mol×K	799.73	Joback Method
cpg	843.80	J/mol×K	771.68	Joback Method
cpg	826.65	J/mol×K	743.63	Joback Method
cpg	808.70	J/mol×K	715.58	Joback Method
cpg	890.54	J/mol×K	855.83	Joback Method

dvisc	0.0000953	Paxs	687.53	Joback Method
dvisc	0.0001278	Paxs	633.74	Joback Method
dvisc	0.0001809	Paxs	579.95	Joback Method
dvisc	0.0002749	Paxs	526.15	Joback Method
dvisc	0.0004595	Paxs	472.36	Joback Method
dvisc	0.0008765	Paxs	418.57	Joback Method
dvisc	0.0020226	Paxs	364.78	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=C2306925&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2306925&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>

## 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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