

# 3-Octenoic acid, heptyl ester

<b>Inchi:</b>	InChI=1S/C15H28O2/c1-3-5-7-9-11-13-15(16)17-14-12-10-8-6-4-2/h9,11H,3-8,10,12-14H
<b>InchiKey:</b>	UVNAAJIDJCCSLH-PKNBQFBNSA-N
<b>Formula:</b>	C15H28O2
<b>SMILES:</b>	CCCCC=CCC(=O)OCCCCCCC
<b>Mol. weight [g/mol]:</b>	240.38

## Physical Properties

Property code	Value	Unit	Source
gf	-78.28	kJ/mol	Joback Method
hf	-480.51	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	58.10	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.636		Crippen Method
mvol	225.350	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	623.05	K	Joback Method
tc	796.03	K	Joback Method
tf	325.89	K	Joback Method
vc	0.879	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.59	J/molxK	623.05	Joback Method
cpg	617.60	J/molxK	651.88	Joback Method
cpg	633.86	J/molxK	680.71	Joback Method
cpg	649.40	J/molxK	709.54	Joback Method
cpg	664.23	J/molxK	738.37	Joback Method
cpg	678.37	J/molxK	767.20	Joback Method
cpg	691.85	J/molxK	796.03	Joback Method
dvisc	0.0024199	Paxs	325.89	Joback Method

dvisc	0.0010480	Paxs	375.42	Joback Method
dvisc	0.0005516	Paxs	424.94	Joback Method
dvisc	0.0003319	Paxs	474.47	Joback Method
dvisc	0.0002199	Paxs	524.00	Joback Method
dvisc	0.0001564	Paxs	573.52	Joback Method
dvisc	0.0001174	Paxs	623.05	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=U406127&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406127&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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