

# Heptanoic acid, hexyl ester

<b>Other names:</b>	hexyl heptanoate
<b>Inchi:</b>	InChI=1S/C13H26O2/c1-3-5-7-9-11-13(14)15-12-10-8-6-4-2/h3-12H2,1-2H3
<b>InchiKey:</b>	IFOGOHVJHKKYCT-UHFFFAOYSA-N
<b>Formula:</b>	C13H26O2
<b>SMILES:</b>	CCCCCOC(=O)CCCCCC
<b>Mol. weight [g/mol]:</b>	214.34
<b>CAS:</b>	1119-06-8

## Physical Properties

Property code	Value	Unit	Source
gf	-175.34	kJ/mol	Joback Method
hf	-556.45	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1699.00		NIST Webbook
tb	534.04 ± 0.30	K	NIST Webbook
tc	741.92	K	Joback Method
tf	225.30 ± 0.50	K	NIST Webbook
vc	0.787	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/molxK	573.13	Joback Method
cpg	531.11	J/molxK	601.26	Joback Method
cpg	546.77	J/molxK	629.39	Joback Method
cpg	561.79	J/molxK	657.52	Joback Method

cpg	576.19	J/mol×K	685.66	Joback Method
cpg	589.97	J/mol×K	713.79	Joback Method
cpg	603.14	J/mol×K	741.92	Joback Method
dvisc	0.0029408	Paxs	308.43	Joback Method
dvisc	0.0013589	Paxs	352.55	Joback Method
dvisc	0.0007456	Paxs	396.66	Joback Method
dvisc	0.0004613	Paxs	440.78	Joback Method
dvisc	0.0003115	Paxs	484.90	Joback Method
dvisc	0.0002245	Paxs	529.01	Joback Method
dvisc	0.0001702	Paxs	573.13	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51239e+01
Coeff. B	-4.66862e+03
Coeff. C	-8.96440e+01
Temperature range (K), min.	404.32
Temperature range (K), max.	565.43

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119068&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119068&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>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>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	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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