

# Octanoic acid, hexyl ester

<b>Other names:</b>	Hexyl caprylate Hexyl octanoate Hexyl octylate n-Hexyl caprylate
<b>Inchi:</b>	InChI=1S/C14H28O2/c1-3-5-7-9-10-12-14(15)16-13-11-8-6-4-2/h3-13H2,1-2H3
<b>InchiKey:</b>	PBGWNXWNCSSXCO-UHFFFAOYSA-N
<b>Formula:</b>	C14H28O2
<b>SMILES:</b>	CCCCCCCC(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	228.37
<b>CAS:</b>	1117-55-1

## Physical Properties

Property code	Value	Unit	Source
gf	-166.92	kJ/mol	Joback Method
hf	-577.09	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.470		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	1564.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1581.90		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1567.00		NIST Webbook

ripol	1565.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1804.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1800.00		NIST Webbook
tb	550.59 ± 0.40	K	NIST Webbook
tc	764.02	K	Joback Method
tf	319.70	K	Joback Method
vc	0.844	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.02	J/mol×K	596.01	Joback Method
cpg	583.90	J/mol×K	624.01	Joback Method
cpg	600.10	J/mol×K	652.01	Joback Method
cpg	615.63	J/mol×K	680.02	Joback Method
cpg	630.49	J/mol×K	708.02	Joback Method
cpg	644.71	J/mol×K	736.02	Joback Method
cpg	658.29	J/mol×K	764.02	Joback Method
dvisc	0.0027735	Paxs	319.70	Joback Method
dvisc	0.0012632	Paxs	365.75	Joback Method
dvisc	0.0006860	Paxs	411.80	Joback Method
dvisc	0.0004212	Paxs	457.86	Joback Method
dvisc	0.0002827	Paxs	503.91	Joback Method
dvisc	0.0002029	Paxs	549.96	Joback Method
dvisc	0.0001532	Paxs	596.01	Joback Method

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51317e+01
Coeff. B	-4.79816e+03
Coeff. C	-9.42030e+01
Temperature range (K), min.	417.44
Temperature range (K), max.	582.80

## 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=C1117551&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1117551&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>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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