

# Hexanoic acid, hexyl ester

<b>Other names:</b>	Hexyl caproate Hexyl hexanoate Hexyl hexoate Hexyl n-hexanoate n-Hexyl caproate n-Hexyl hexanoate n-Hexyl n-hexanoate
<b>Inchi:</b>	InChI=1S/C12H24O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h3-11H2,1-2H3
<b>InchiKey:</b>	NCDCLPBOMHPFCV-UHFFFAOYSA-N
<b>Formula:</b>	C12H24O2
<b>SMILES:</b>	CCCCCOC(=O)CCCC
<b>Mol. weight [g/mol]:</b>	200.32
<b>CAS:</b>	6378-65-0

## Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-535.81	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	51.46	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1385.00		NIST Webbook
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rinpol	1356.00	NIST Webbook
rinpol	1368.00	NIST Webbook
rinpol	1390.00	NIST Webbook
rinpol	1371.00	NIST Webbook
rinpol	1376.00	NIST Webbook
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rinpol	1378.00	NIST Webbook
rinpol	1393.00	NIST Webbook
rinpol	1384.00	NIST Webbook
rinpol	1384.00	NIST Webbook
rinpol	1371.00	NIST Webbook
rinpol	1383.00	NIST Webbook
rinpol	1353.00	NIST Webbook
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ripol	1619.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1612.00		NIST Webbook
tb	518.58 ± 0.30	K	NIST Webbook
tc	720.05	K	Joback Method
tf	217.90 ± 0.40	K	NIST Webbook
tt	217.00	K	Heat capacities of potential organic phase change materials
vc	0.732	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.22	J/mol×K	720.05	Joback Method
cpg	479.84	J/mol×K	578.55	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	509.36	J/mol×K	635.15	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	464.17	J/mol×K	550.25	Joback Method

dvisc	0.0030867	Paxs	297.16	Joback Method
dvisc	0.0014485	Paxs	339.34	Joback Method
dvisc	0.0008035	Paxs	381.52	Joback Method
dvisc	0.0005012	Paxs	423.70	Joback Method
dvisc	0.0003406	Paxs	465.89	Joback Method
dvisc	0.0002467	Paxs	508.07	Joback Method
dvisc	0.0001878	Paxs	550.25	Joback Method
pvap	3.13e-03	kPa	298.40	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	4.90e-03	kPa	303.20	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	7.32e-03	kPa	308.00	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.01	kPa	312.80	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.01	kPa	312.80	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.02	kPa	317.70	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.03	kPa	322.60	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.04	kPa	327.50	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction

pvap	0.05	kPa	332.40	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.08	kPa	337.30	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.11	kPa	342.30	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.14	kPa	347.30	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.15	kPa	347.30	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51432e+01
Coeff. B	-4.55839e+03
Coeff. C	-8.54740e+01
Temperature range (K), min.	392.32
Temperature range (K), max.	549.11

## Sources

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6378650&Units=SI>

**The Yaws Handbook of Vapor**

**Pressure:**  
**Crippen Method:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Heat capacities of potential organic**

**phase change materials:**

**Biomass Valorization:**

**Thermodynamics of the Guerbet**

**Condensation Reaction:**

<https://www.doi.org/10.1016/j.jct.2018.08.014>

<https://www.doi.org/10.1021/acs.jced.9b00419>

## 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>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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