

# Hydroperoxide, heptyl

<b>Other names:</b>	Heptyl hydroperoxide 1-Heptyl hydroperoxide 1-Hydroperoxyheptane n-C7H15OOH
<b>Inchi:</b>	InChI=1S/C7H16O2/c1-2-3-4-5-6-7-9-8/h8H,2-7H2,1H3
<b>InchiKey:</b>	XIOGAMSYSPUSI-UHFFFAOYSA-N
<b>Formula:</b>	C7H16O2
<b>SMILES:</b>	CCCCC(O)O
<b>Mol. weight [g/mol]:</b>	132.20
<b>CAS:</b>	764-81-8

## Physical Properties

Property code	Value	Unit	Source
chl	-4698.20 ± 5.00	kJ/mol	NIST Webbook
gf	-335.85	kJ/mol	Joback Method
hf	-538.08	kJ/mol	Joback Method
hfus	24.03	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
ie	9.48 ± 0.03	eV	NIST Webbook
ie	9.88	eV	NIST Webbook
log10ws	-2.15		Crippen Method
logp	2.446		Crippen Method
mvol	121.230	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	505.07	K	Joback Method
tc	691.97	K	Joback Method
tf	329.25	K	Joback Method
vc	0.452	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.89	J/mol×K	505.07	Joback Method
cpg	278.91	J/mol×K	536.22	Joback Method

cpg	289.41	J/molxK	567.37	Joback Method
cpg	299.40	J/molxK	598.52	Joback Method
cpg	308.91	J/molxK	629.67	Joback Method
cpg	317.95	J/molxK	660.82	Joback Method
cpg	326.55	J/molxK	691.97	Joback Method
dvisc	0.0017830	Paxs	329.25	Joback Method
dvisc	0.0011581	Paxs	358.55	Joback Method
dvisc	0.0008029	Paxs	387.86	Joback Method
dvisc	0.0005860	Paxs	417.16	Joback Method
dvisc	0.0004458	Paxs	446.46	Joback Method
dvisc	0.0003507	Paxs	475.77	Joback Method
dvisc	0.0002837	Paxs	505.07	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=C764818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C764818&amp;Units=SI</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<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>ie:</b>	Ionization energy
<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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point

**vc:** Critical Volume

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