

# Hydroperoxide, 1-ethylbutyl

<b>Other names:</b>	3-Hexyl hydroperoxide 1-Ethylbutyl hydroperoxide 3-Hydroperoxyhexane
<b>Inchi:</b>	InChI=1S/C6H14O2/c1-3-5-6(4-2)8-7/h6-7H,3-5H2,1-2H3
<b>InchiKey:</b>	NMNOLZYZNVYLRJ-UHFFFAOYSA-N
<b>Formula:</b>	C6H14O2
<b>SMILES:</b>	CCCC(CC)OO
<b>Mol. weight [g/mol]:</b>	118.17
<b>CAS:</b>	24254-56-6

## Physical Properties

Property code	Value	Unit	Source
chl	-4057.00	kJ/mol	NIST Webbook
gf	-244.62	kJ/mol	Joback Method
hf	-456.90	kJ/mol	Joback Method
hfus	13.05	kJ/mol	Joback Method
hvap	47.65	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	2.055		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	965.00		NIST Webbook
rinpol	965.00		NIST Webbook
tb	450.84	K	Joback Method
tc	615.45	K	Joback Method
tf	225.43	K	Joback Method
vc	0.403	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.32	J/mol×K	450.84	Joback Method
cpg	239.95	J/mol×K	478.28	Joback Method
cpg	249.26	J/mol×K	505.71	Joback Method

cpg	258.28	J/mol×K	533.15	Joback Method
cpg	266.99	J/mol×K	560.58	Joback Method
cpg	275.39	J/mol×K	588.02	Joback Method
cpg	283.50	J/mol×K	615.45	Joback Method
dvisc	0.0820702	Paxs	225.43	Joback Method
dvisc	0.0143235	Paxs	263.00	Joback Method
dvisc	0.0038675	Paxs	300.57	Joback Method
dvisc	0.0013969	Paxs	338.13	Joback Method
dvisc	0.0006185	Paxs	375.70	Joback Method
dvisc	0.0003176	Paxs	413.27	Joback Method
dvisc	0.0001822	Paxs	450.84	Joback Method

## Sources

<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=C24254566&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C24254566&amp;Units=SI</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>

## 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>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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