

# Hexyl octyl ether

<b>Inchi:</b>	InChI=1S/C14H30O/c1-3-5-7-9-10-12-14-15-13-11-8-6-4-2/h3-14H2,1-2H3
<b>InchiKey:</b>	KUTWKGLRMXBROO-UHFFFAOYSA-N
<b>Formula:</b>	C14H30O
<b>SMILES:</b>	CCCCCCCCOCCCCC
<b>Mol. weight [g/mol]:</b>	214.39
<b>CAS:</b>	17071-54-4

## Physical Properties

Property code	Value	Unit	Source
gf	-38.00	kJ/mol	Joback Method
hf	-464.51	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.944		Crippen Method
mcvol	213.990	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
tb	530.70 ± 2.00	K	NIST Webbook
tc	701.88	K	Joback Method
tf	246.20 ± 1.50	K	NIST Webbook
vc	0.838	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.33	J/mol×K	542.14	Joback Method
cpg	554.10	J/mol×K	568.76	Joback Method
cpg	571.22	J/mol×K	595.39	Joback Method
cpg	587.72	J/mol×K	622.01	Joback Method
cpg	603.58	J/mol×K	648.63	Joback Method
cpg	618.84	J/mol×K	675.26	Joback Method
cpg	633.50	J/mol×K	701.88	Joback Method
dvisc	0.0038629	Paxs	269.77	Joback Method
dvisc	0.0015169	Paxs	315.16	Joback Method

dvisc	0.0007537	Paxs	360.56	Joback Method
dvisc	0.0004379	Paxs	405.95	Joback Method
dvisc	0.0002838	Paxs	451.35	Joback Method
dvisc	0.0001991	Paxs	496.75	Joback Method
dvisc	0.0001482	Paxs	542.14	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C17071544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C17071544&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>
<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>mccvol:</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
<b>vc:</b>	Critical Volume

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