

# Hexane, 1-ethoxy-

Other names:	1-ethoxyhexane 3-oxanonane ether, ethyl hexyl ethyl hexyl ether ethyl n-hexyl ether hexyl ethyl ether
Inchi:	InChI=1S/C8H18O/c1-3-5-6-7-8-9-4-2/h3-8H2,1-2H3
InchiKey:	ZXHQLEQLZPJIFG-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCCCCOC
Mol. weight [g/mol]:	130.23
CAS:	5756-43-4

## Physical Properties

Property code	Value	Unit	Source
gf	-88.52	kJ/mol	Joback Method
hf	-340.67	kJ/mol	Joback Method
hfus	17.66	kJ/mol	Joback Method
hvap	35.81	kJ/mol	Joback Method
ie	9.33	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	2.603		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	882.00		NIST Webbook
rinpol	882.00		NIST Webbook
tb	404.86	K	Joback Method
tc	568.81	K	Joback Method
tf	202.15	K	Joback Method
vc	0.501	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	257.48	J/molxK	404.86	Joback Method
cpg	327.83	J/molxK	568.81	Joback Method
cpg	282.47	J/molxK	459.51	Joback Method
cpg	294.38	J/molxK	486.84	Joback Method
cpg	305.91	J/molxK	514.16	Joback Method
cpg	317.06	J/molxK	541.49	Joback Method
cpg	270.17	J/molxK	432.19	Joback Method
dvisc	0.0002873	Paxs	371.08	Joback Method
dvisc	0.0003956	Paxs	337.29	Joback Method
dvisc	0.0005852	Paxs	303.50	Joback Method
dvisc	0.0009546	Paxs	269.72	Joback Method
dvisc	0.0017915	Paxs	235.94	Joback Method
dvisc	0.0002200	Paxs	404.86	Joback Method
dvisc	0.0041498	Paxs	202.15	Joback Method
rhoI	745.27	kg/m3	323.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model
rhoI	749.66	kg/m3	318.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model
rhoI	754.06	kg/m3	313.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model
rhoI	762.80	kg/m3	303.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model

rho_l	767.15	kg/m3	298.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model
rho_l	771.47	kg/m3	293.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model
rho_l	775.80	kg/m3	288.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model
rho_l	758.45	kg/m3	308.15	Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model

Sources

Crippen Method:

Crippen Method:

Liquid-liquid equilibrium in binary systems of isomeric C8 aliphatic monoethers with acetonitrile

Excess Enthalpies in Binary Systems of Isomeric C8 Aliphatic Monoethers with Acetonitrile and Their Description by the COSMO-SAC Model:

McGowan Method:

NIST Webbook:

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

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

<https://www.doi.org/10.1016/j.fluid.2013.07.002>

<https://www.doi.org/10.1016/j.jct.2014.12.025>

<https://www.doi.org/10.1021/acs.jced.5b00838>

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

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5756434&Units=SI>

# 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>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>rho:</b>	Liquid Density
<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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