

# Hexane, 1,1-diethoxy-

<b>Other names:</b>	Hexanal, diethyl acetal 1,1-Diethoxyhexane n-Hexanal diethyl acetal
<b>Inchi:</b>	InChI=1S/C10H22O2/c1-4-7-8-9-10(11-5-2)12-6-3/h10H,4-9H2,1-3H3
<b>InchiKey:</b>	WNHOMUCDFNTSEV-UHFFFAOYSA-N
<b>Formula:</b>	C10H22O2
<b>SMILES:</b>	CCCCCC(OCC)OCC
<b>Mol. weight [g/mol]:</b>	174.28
<b>CAS:</b>	3658-93-3

## Physical Properties

Property code	Value	Unit	Source
gf	-179.12	kJ/mol	Joback Method
hf	-519.45	kJ/mol	Joback Method
hfus	20.51	kJ/mol	Joback Method
hvap	42.29	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.966		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
ripol	1092.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1080.00		NIST Webbook
ripol	1082.00		NIST Webbook
ripol	1087.90		NIST Webbook
ripol	1242.00		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1227.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1227.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1227.00		NIST Webbook
ripol	1229.00		NIST Webbook

ripol	1235.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1223.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1242.00		NIST Webbook
tb	472.60	K	Joback Method
tc	638.49	K	Joback Method
tf	231.92	K	Joback Method
vc	0.625	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.40	J/molxK	472.60	Joback Method
cpg	439.18	J/molxK	610.84	Joback Method
cpg	426.16	J/molxK	583.19	Joback Method
cpg	412.67	J/molxK	555.54	Joback Method
cpg	398.71	J/molxK	527.90	Joback Method
cpg	384.29	J/molxK	500.25	Joback Method
cpg	451.74	J/molxK	638.49	Joback Method
dvisc	0.0001614	Paxs	472.60	Joback Method
dvisc	0.0002182	Paxs	432.49	Joback Method
dvisc	0.0003135	Paxs	392.37	Joback Method
dvisc	0.0004893	Paxs	352.26	Joback Method
dvisc	0.0008564	Paxs	312.15	Joback Method
dvisc	0.0017676	Paxs	272.03	Joback Method
dvisc	0.0046878	Paxs	231.92	Joback Method

## Sources

**McGowan Method:**

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

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3658933&Units=SI>

**Crippen Method:**

<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)

**Joback Method:**

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

# 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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