Hexane, 1,1'-oxybis-

Other names:	1-(Hexyloxy)hexane
	7-oxatridecane
	BIS(1-HEXYL)ETHER
	DIHEXYLETHER
	Di-n-hexyl ether
	Dihexyl ether
	Ether, dihexyl
	Hexyl ether
	n-Hexyl ether
Inchi:	InChI=1S/C12H26O/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-12H2,1-2H3
InchiKey:	BPIUIOXAFBGMNB-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CCCCCCOCCCCCC
Mol. weight [g/mol]:	186.33
CAS:	112-58-3

Physical Properties

Property code	Value	Unit	Source
af	0.7000		KDB
gf	-54.84	kJ/mol	Joback Method
hf	-423.23	kJ/mol	Joback Method
hfus	28.02	kJ/mol	Joback Method
hvap	63.60 ± 0.80	kJ/mol	NIST Webbook
hvap	64.10 ± 0.10	kJ/mol	NIST Webbook
hvap	63.50	kJ/mol	NIST Webbook
hvap	64.10	kJ/mol	NIST Webbook
log10ws	-3.93		Crippen Method
logp	4.164		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1820.00	kPa	KDB
rinpol	1228.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1287.00		NIST Webbook

ripol	1367.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1349.00		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1368.00		NIST Webbook
tb	499.60	K	KDB
tb	501.70	K	NIST Webbook
tc	657.00	K	KDB
tc	665.00	K	Critical properties of some aliphatic symmetrical ethers
tf	230.00	K	KDB
vc	0.720	m3/kmol	KDB
zc	0.2398840		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.65	J/mol×K	496.38	Joback Method
cpg	452.08	J/mol×K	523.22	Joback Method
cpg	467.95	J/mol×K	550.06	Joback Method
cpg	483.25	J/mol×K	576.89	Joback Method
cpg	497.99	J/mol×K	603.73	Joback Method
cpg	512.19	J/mol×K	630.57	Joback Method
cpg	525.85	J/mol×K	657.41	Joback Method
dvisc	0.0016995	Pa×s	288.75	Joback Method
dvisc	0.0042171	Pa×s	247.23	Joback Method
dvisc	0.0008607	Pa×s	330.28	Joback Method
dvisc	0.0005075	Pa×s	371.80	Joback Method
dvisc	0.0003327	Pa×s	413.33	Joback Method
dvisc	0.0002356	Pa×s	454.86	Joback Method
dvisc	0.0001768	Pa×s	496.38	Joback Method
hvapt	52.90	kJ/mol	441.00	NIST Webbook
rhol	794.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52361e+01
Coeff. B	-4.47931e+03
Coeff. C	-7.98300e+01
Temperature range (K), min.	379.48
Temperature range (K), max.	531.16

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.36877e+02
Coeff. B	-1.28585e+04
Coeff. C	-1.74530e+01
Coeff. D	7.82721e-06
Temperature range (K), min.	230.15
Temperature range (K), max.	658.00

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Critical properties of some aliphatic symmetrical ethers: https://www.doi.org/10.1016/j.jct.2013.09.019

KDB: https://www.cheric.org/files/research/kdb/mol/mol1025.mol

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1025

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112583&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility